UNIVERSITY OF PARDUBICE
Faculty of Chemical Technology

Department of Theory and Technology of Explosives

NEW TRENDS IN RESEARCH OF ENERGETIC MATERIALS

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Content

DISLOCATION - ASSISTED INITIATION OF ENERGETIC MATERIALS

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Abstract
The role of dislocations in assisting initiation of (explosive) chemical decomposition of energetic materials has connection with the known influences for crystals and polycrystals of dislocations facilitating permanent deformations and phase transformations. X-ray topographic observation of relatively few dislocations in solution-grown crystals relates to the influence of large Burgers (displacement) vectors that are characteristic of molecular crystal bonding. Both model evaluations of the load dependence of cracking at hardness indentations and the derived hardness stress-strain behaviors show that dislocation movement is difficult whether in the indentation strain fields or at the tips of indentation-induced cracks. Thus, energetic crystals are elastically compliant, plastically hard, and relatively brittle [1]. Nevertheless, cracking is shown to be facilitated by the shear stress driven, normally limited, dislocation flow that, on molecular dynamics and dislocation pile-up model bases, is shown to be especially prone to producing localized hot spot heating for explosive initiations. Such model consideration is in agreement with greater drop-weight heights being required to initiate smaller crystals. The crystal size effect carries over to more difficult combustion occurring for compaction of smaller crystals. The total results relate to dual advantages of greater strength and reduced mechanical sensitivity accruing for the development of nanocrystal formulations. In consequence, also, several levels of dislocation-assisted modeling are described for initiation mechanisms under shock wave loading conditions.
NTREM, PARDUBICE, 2005 page 32-47

A QUANTUM CHEMICAL STUDY ON THERMOLYSIS INITIATION MECHANISMS AND IMPACT SENSITIVITY OF ENERGETIC MATERIALS

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Abstract:
Thermolysis initiation mechanisms of polynitro compounds, tetrazole derivatives and their metallic salts, and cage high energy density compounds have been investigated using quantum chemical approaches. Our calculations show that the trigger bonds whose breaking initiate a decomposition or an explosion are C-NO_2 or N-NO_2 bonds for nitro derivatives of benzene and aminobenzenes, CL-20 and polynitroadamantanes. Explosion of nitro derivatives of phenol and toluene are most likely triggered by the isomerization reactions involving the H-shift. Due to larger strain energy, the trigger bond is found to be the C-C bond in the framework of polynitrocubanes. Regarding tetrazoles and their metallic salts, opening of the tetrazole ring, i.e., scission of the N-N bond, followed by formation ofN2 molecules, initiate explosive reactions. We found for energetic materials having similar molecular structures and following similar thermal decomposition mechanisms, the bond orders of the trigger bond and the activation energy to break the bond are directly related to the impact sensitivity. We thus proposed two criteria used to evaluate the relative ordering of impact sensitivity of energetic materials with similar structures: the smaller the bond order, the more sensitive an energetic material, which is called the principle of the smallest bond order (PSBO). And the higher the activation energy, the less sensitive a material. We demonstrated that in most cases the principle of the smallest bond order (PSBO) is equivalent to the activation energy criterion. The former is more convenient and easier to obtain while the latter can be applied more
NTREM, PARDUBICE, 2005 page 48-62

SOME NOTES ON THE FUNDAMENTALS OF E.M. INITIATION Towards a "UNIVERSAL SENSITIVITY CHARACTERISTIC"?

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Abstract:

The stimulus needed for initiation of an energetic material is an important quantity to determine for reliable functioning and safe handling. When considering the gamma of impact, friction, spark and heating tests in use one runs into the problem of how to compare results and how to make a prediction for practical situations that an initiation certainly will happen or definitely can be excluded. The way forward is not easy. The initiation process, which in order to be successful, should be followed by sustained propagation, is not simply accessible. This paper tries to produce a contribution by considering the fundamental aspects and to show as an example some simulation results of a gas phase initiation model. Some suggestions are made for making further progress.

NTREM, PARDUBICE, 2005 page 63-73

ATOMISTIC STUDIES OF FUNDAMENTAL PROPERTIES AND PROCESSES IN ENERGETIC MATERIALS: RELEVANCE TO MESOSCALE INITIATION PHENOMENA

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Abstract:

Genuine, physics-based understanding of initiation phenomena in plastic-bonded explosives (PBXs) requires knowledge of the physics and chemistry at mesoscopic scales that are far larger than can be simulated directly using atomistic detail, yet far smaller than is directly resolvable in practical engineering scale continuum simulations. Initiation is determined by localization phenomena that arise due to the heterogeneous character of most explosive formulations. Indeed, the "average" temperature behind a weak shock is not a useful measure for understanding initiation phenomena; rather, it is the tails of the distributions in temperature, stress, and strain rates, localized to small, spatially distributed volumes in the material (hot spots), that dictate the outcome of a given loading event.

Important factors for predicting hot spot formation and subsequent extinction or growth/coalescence include particle size, concentration, morphology, and void content; physical and chemical interactions between grains and binder; thermophysical and mechanical properties of the constituents and interfaces between them; and, of course, the inherent chemical stability of the explosive component(s) in the formulation. We are in the process of computing many of the thermophysical and mechanical properties required for a complete specification of constituent models for use in mesoscale simulations, wherein grains and binder in representative volumes of a PBX are spatially resolved and then studied within a continuum hydrodynamic framework. In addition to calculating specific properties of interest, we have recently undertaken a series of large-scale molecular dynamics simulations of energetic crystals to understand dissipation phenomena in dynamically loaded single- or poly-crystalline samples; for instance, plastic deformation and stress/energy localization mechanisms, phase transitions, and so on. Recent and ongoing work in these areas will be discussed, along with their specific relevance to emerging mesoscale simulation capabilities.

NTREM, PARDUBICE, 2005 page 74-90

HIGH-TEMPERATURE PROPELLANT TORCH-SYSTEM FOR NON-DETONATIVE NEUTRALIZATION OF MINES; SOME PHYSICAL AND CHEMICAL ASPECTS

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Abstract:
A novel, proprietary "rocket-type" torch, using very-high-temperature pyrotechnic and propellant compositions initially developed at IIT Research Institute (IITRI) under U.S. Government contract, has been extensively further developed and demonstrated in recent years at Applied Research Associates, Inc. (ARA) to be effective in penetrating all explosive mines and neutralizing all mine explosive types tested without causing the explosive to detonate. This ARA proprietary PTS torch is based mainly on the use of aluminum and potassium perchlorate to optimize its temperatue and performance; the computed chamber temperatures are in excess of 4000 ^{o}K. Total torch burning times are generally in excess of 30 sec, although penetrations of thick steel are within a few sec, mandatory for the penetration of steel casings since long penetration times cause excessive heating of the steel which can prevent penetration as well as allow the buildup of slag and other solid condensables from the torch products that can interfere with the subsequent capability of igniting the explosive. The long burn time of the torch after penetration is required to assure adequate ignition of the explosive, particularly TNT. A similar but more robust and heavier torch developed in Russia at the Semenov Institute of Chemical Physics (SICP) of the Russian Academy of Sciences penetrates 25mm steel within seconds (Ref 1). This earlier effort emphasized the penetration of thick steel, wood, and thermoplastics of surface exposed mines, the so-called "hardened mines ". This work has now been extended to mines that are covered with water and/or soil, to the extent encountered in the Global Humanitarian Demining Program. Work involving mines under water and/or soil is currently underway by the U.S, Government; some work conducted under IR&D in the U.S. at. ARA as well as at SICP is described here, with emphasis on the physical and chemical aspects of neutralizing the explosive within the mine after penetration of the casing is achieved. In particular, because of its inadequate oxidizer balance, TNT is very difficult to initiate and achieve sustained autocatalytic decomposition when attempted under conditions wherein air (oxygen) is inadequate or absent; e.g., underwater and underground. When burned in open air, TNT decomposes/combusts but still provides voluminous black smoke due to inadequate combustion of carbon.
NTREM, PARDUBICE, 2005 page 91-99

HIGHLIGHTS OF STABILITY RESEARCH IN THE FIRST DOZEN OF JAN HANSSON SYMPOSIA 1967 - 2001

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Abstract
This paper is dealing with a review of reports on chemical stability of propellants presented in the first Twelve Jan Hansson Symposia (S1 - S12) on Chemical Problems Connected with the Stability of Explosives 1967 - 2001.
NTREM, PARDUBICE, 2005 page 100-118

LIABILITY OF AMMONIUM NITRATE EMULSIONS TO SPONTANEOUS DECOMPOSITION

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Abstract:
Thermal properties of some ammonium nitrate emulsions were investigated by means of a heat flow calorimeter SETARAM C80D. Kinetic parameters of ammonium nitrate emulsions like activation energy, frequency factor were determined. Based on these data, applying Frank-Kamenetskii's model, the critical radius and temperature for a sphere were estimated.
NTREM, PARDUBICE, 2005 page 119-129

COMPUTER SIMULATION OF NITRO-1,2,4-TRIAZOLES DECOMPOSITION REACTIONS

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Abstract:
The combination of nitro-groups with polynitrogenous heterocycles and, in particular, with 1,2,4-triazoles is often used for the synthesis of power-consuming compounds. For these materials creation, an advance estimation of the basic characteristics is crucial to select the most prospective structures for subsequent synthesis. One of the most important characteristics of power-consuming compounds is the thermal stability connected with the processes of thermal decomposition. Nevertheless, nowadays a theoretical description of multi-channel process of decomposition represents a complicated problem and has been mainly limited by the primary decomposition act with simplified schemes of the process.
On the basis of Recombination Reaction Networks, a stringent approach to the generation of a set of hypotheses for the mechanism of thermolysis has been elaborated. In this work, our methodology has been used for computer simulation of decomposition reactions ofN-nitro and C-nitro-1,2,4-triazoles. Subsequent estimation of the thermo-chemical preference of these or other decomposition pathways has been estimated using DFTB3LYP 6-31G method. The schemes obtained have been collated with the available experimental data.*
NTREM, PARDUBICE, 2005 page 130-137

BOMB CALORIMETRIC STUDY OF A SERIES OF ENERGETIC LINEAR POLYPHOSPHAZENES

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Abstract:
Energetic linear polyphosphazenes are of potential interest as novel binders for energetic formulations. However, the presence of phosphorus in these materials renders their combustion chemistry significantly different to that of conventional binders. This paper explores the combustion chemistry of a series of energetic polyphosphazenes. The heat of combustion of each member of the series has been measured by bomb calorimetry, and the water-soluble combustion products have been identified and quantified using NMR Spectroscopy and Ion Chromatography. Since some of the combustion products are hydrolytically unstable, it was necessary to stabilise the initial combustion product mixtures by using a buffer solution instead of pure water in the bomb, and then to determine the composition of the stabilized product mixtures in order to obtain meaningful values for the heats of combustion and thence heats of formation. The thermochemical measurements themselves were made with pure water in the bomb. The composition and structures of the various polyphosphazenes have been correlated with their heats of combustion and should enable polyphosphazenes with specific thermochemical properties to be identified. The 'combustion' of the polyphosphazenes under a nitrogen atmosphere has also been studied.
NTREM, PARDUBICE, 2005 page 138-145

DETERMINATION OF POST-EXPLOSION RESIDUES OF AMMONIUM NITRATE IN ENVIRONMENTAL SAMPLES

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Abstract:
The paper presents results of determination of ammonium nitrate, which remains in detonation products of industrial explosives. Charges of the explosives containing ammonium nitrate were detonated inside samples of concrete, sand and wood. After detonation, we tried to detect ammonium nitrate in the matrixes using instrumental thin layer chromatography (TLC). In this way a possibility of identification and determination of ammonium nitrate on the spot of criminal events was confirmed.
NTREM, PARDUBICE, 2005 page 146-150

REACTIVITY BETWEEN ε-CL20-GAP AND β-HMX-GAP INVESTIGATED BY MASS LOSS, ADIABATIC SELF HEATING AND DYNAMIC MECHANICAL ANALYSIS

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Abstract
The crystalline energetic component ε-CL20 (ε-HNIW, hexanitro-hexaaza-isowurtzitane, crystallized in ε-phase) has the potential to be used as ingredient in high performance formulations, for example in high burning rate rocket propellants. A closer inspection of the reactivity of ε-CL20 revealed a marked difference between ε-CL20-GAP and β-HMX-GAP. Experimental data of the reactivity between the 1:1 by mass mixtures ε-CL20-GAP diol, β-HMX-GAP diol and of 45:55 by mass formulations ε-CL20/GAP-N100 and β-HMX/GAP-N100 (GAP-N100 means GAP diol cured with Desmodur^{T}M N100) are presented. The data have been obtained by the following measurement methods:

- *mass loss*
- *gas generation*
- *adiabatic self heat rate measured by ARC^{T}M*
- *dynamic mechanical analysis (DMA)*

Gas generation determined with a standard vacuum stability test apparatus was used to sustain the evaluation. With all four measurement methods the difference in reactivity between ε-CL20-GAP and β-HMX-GAP is found. Further to this a difference in reactivity is observed between the mere mixture of ε-CL20-GAP diol and the 45:55 formulation ε-CL20/GAP-N100. So-named reactivity functions are obtained from the raw data of mass loss, which describe the reactive part between the components. The investigation of the mechanical properties of the 45:55 formulations ε-CL20/GAP-N100 and β-HMX/GAP-N100 by dynamic mechanical analysis shows the marked difference in binder ageing between them.

NTREM, PARDUBICE, 2005 page 151-178

DETONATION VELOCITY OF EMULSION EXPLOSIVES WITH CENOSPHERES

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Abstract:
The velocity of detonation of emulsion explosive with microspheres from coal ash (cenospheres) was measured. The diameter of cenospheres was changed from 50 to 250 microns. The comparison of the dependence of detonation velocity vs. density and diameter of charge with different sensitizers was carried out. The maximal detonation velocity for cenospheres 70 -100 micron fraction was determined to be 5.5 - 5.6 km/s. This value of detonation velocity is equal to the maximal detonation velocity determined for the charges of emulsion with glass microballoons produced by 3M Company [1]. The critical diameter for the charge with cenospheres was determined as 35 - 40 mm to be 1.5 - 2 times more than that of for the charge with 3M microballoons.

NTREM, PARDUBICE, 2005 page 179-183

SYNTHESIS AND CHARACTERISATION OF 2,2-DINITRO-1,3-PROPANEDIOL-BASED PLASTICISERS

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Abstract:

In this paper, the synthesis of two energetic plasticisers (2,2-dinitro-1,3-bis(2-azido acetoxy) propane and 2,2-dinitro-1,3-bis(formyloxy)propane) and the attempted syntheses of even further derivatives are described. The prepared compounds were characterised and evaluated as plasticisers. Their glass transition temperatures are acceptable to excellent, but both of them are thermally unstable.

NTREM, PARDUBICE, 2005 page 184-193

PROPERTIES OF A HIGHLY FRICTION SENSITIVE DERIVATIVE OF 1,5-DIAMINO-1H-TETRAZOLE (DAT): 1,5-DIAMINO-4-METHYLTETRAZOLIUM DINITRAMIDE

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Abstract

The reaction of 1,5-diamino-1H-tetrazole (1) with iodomethane followed by the methathesis of the iodide (2) with silver dinitramide yields the highly friction sensitive 1,5-diamino-4-methyltetrazolium dinitramide (3). 3 crystallize in the orthorhombic space groups $P2_12_12_1$ and shows an intriguing interaction of one nitro group of the dinitramide anion with the tetrazolium cation. Preliminary sensitivity testing of the crystalline compound 3 indicates rather low impact sensitivity with a value of 7 J in contrast to the relatively high friction sensitivity of 24 N. The thermal decomposition of 3 was investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Mass spectrometry and IR spectroscopy were used to identify the gaseous products.

NTREM, PARDUBICE, 2005 page 194-203

STUDY OF NON-ISOTHERMAL NITRIDATION OF ALUMINUM NANOPOWDERS PASSIVATED BY NON-OXIDE LAYERS

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Abstract:
Results ofDTA-TG investigation and chemical analysis of electro-exploded aluminum nanopowders coated and/or passivated with the reactive reagents: nitrocellulose (NC), oleic ($C_{17}H_{33}COOH$) and stearic ($C_{17}H_{35}COOH$) acids, amorphous boron and air (for a comparison) are discussed. Surface protection of aluminum nanopowders by coatings of different origin results in significant advantages in the energetic properties of the powders. Aluminum nanopowders with a protecting surface show increased stability to oxidation during storage period.
NTREM, PARDUBICE, 2005 page 204-210

OPTIMIZATION OF 1,1-DIAMINO-2,2-DINITROETHENE SYNTHESIS

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Abstract:
Known syntheses of 2-methylpyrimidine-4,6(3H,5H)-dione and 1-diamino-2,2-dinitoethene (DADNE), have been studied in order to improve their yield. Parameters affecting yield of both the compound were recognized and optimized. A new method of DADNE stabilization and purification was developed. The overall yield of DADNE synthesis starting from acetamidine hydrochloride was shown to be around 65%.
NTREM, PARDUBICE, 2005 page 211-216

THE INFLUENCE OF THE STRUCTURE OF THE SALTS OF AZOLES UPON THE PROCESSES OF THEIR THERMAL AND LASER INITIATION

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Abstract:
It is experimentally shown that for metal salts of azoles there is no universal factor determining the processes of deflagration under thermal and laser initiation. For the series of azoles having a common initial stage of thermal degradation, the step of deflagration-to-detonation transition (DDT) for the same metal cation depends on Hf_0 value of the salt.
At the same time within the range of silver salts ofisomeric N-nitroaminotetrazoles ΔHf_0 values of the compounds, their structure, reactivity of the products of the initial decomposition and the composition of gaseous products of burning all influence their initiating ability under thermal initiation.
But the ionization potential of complex perchlorates of d-metals with 3(5)-hydrazino-4-amino-1,2,4-triazoles as ligands determines the intensity of initial steps of decomposition under laser initiation which, in its tern controls the threshold of ignition.
Hence the knowledge of the nature of initial decomposition stages of azole salts, taking into account the mechanism of energetic effects, is necessary for prediction of their behavior under initiation.
NTREM, PARDUBICE, 2005 page 217-225

CALCULATIONS OF DENSITIES AND HEATS OF FORMATIONS OF ENERGETIC MOLECULES FOR THE USE IN THERMOCHEMICAL CODES

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Abstract:

Performance of energetic molecules is evaluated by thermo chemical codes which need the input of density, heat of formation and formula. Density and heat of formation for target compounds are values that need to be determined. In this paper two different methods to calculate these values have been applied to a common set of known energetic molecules. These methods are briefly described and the results from these calculations are compared.

NTREM, PARDUBICE, 2005 page 226-235

CHARACTERIZATION OF DETERRED PROPELLANTS BY CLOSED VESSEL TESTS: IMPORTANCE OF THE IGNITION METHOD

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Abstract:

Different gaseous ignition systems have been used for the characterisation of spherical deterred propellants in closed vessel tests. It has been observed that, with an appropriate ignition system, a good correlation is obtained between closed vessel tests, deterrent concentration profiles and ballistic firing.

NTREM, PARDUBICE, 2005 page 236-248

A MOLECULAR DYNAMICS SIMULATION STUDY OF ELASTIC PROPERTIES OF HMX-BASED AND TATB-BASED PBXS

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Abstract:
Three different models, i.e., "inserting", "covering" and "cutting" models, for PBXs were proposed for different researching aspects. Used for choosing polymeric binders, the "inserting" and "covering" models are mainly applied to find the relations of temperatures and concentrations respectively with elastic properties of the PBXs. The "cutting" model is especially used to describe the highly anisotropic behavior of TATB. These models were simulated with molecular dynamics using COMPASS force field. It is found that the mechanical properties of ß-HMX and TATB can be effectively improved by blending fluorine containing polymers in small amount. The moduli of the PBXs decrease with increasing temperature and concentration of binders. Different crystal surfaces interacting with the same polymer binder have different modulus-decreasing effects due to the highly anisotropic behavior of TATB. The modulus-decreasing effect ranking order is (010) . (100) > (001).
NTREM, PARDUBICE, 2005 page 249-259

THE APPLICATION OF A SURFACE ACTIVE THEORY TO ENERGETIC MATERIALS -RESEARCH ON EXPANSION AMMONIUM NITRATE EXPLOSIVES

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Abstract:
The expansion of Ammonium Nitrate(AN)is a novel technology. The guideline of this innovation is the self-sensitization of AN. It is a breakthrough to classic methods. The approach to self-sensitization is the expansion of AN. Its essence is a surfactant technology applied to powdery industrial explosive, and it is a physical and chemical process under coercive crystallization. In this paper, the mechanism and technical characteristics of expansion of AN are discussed and its unique advantage is shown. The expansion technology of AN is mainly applied to rock expanded AN explosive and its comparison with other industry explosives is also given. The expansion technology is also used in manufacturing of permitted explosive and other industrial explosives.
NTREM, PARDUBICE, 2005 page 260-270

CONCEPT OF THE SPATIAL-PERIODIC MICRO-STRUCTURES EXCITATION AT THE EVAPORATED ENERGETIC MATERIALS TRANSIENT COMBUSTION AS A WAY FOR IMPROVEMENT OF THE SOLID PROPULSION TECHNOLOGIES

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Abstract:

In connection with development of solid propulsion systems (SPS) of a new generation with high energy and mass characteristics, the problem of prevention of development of combustion instability and anomalies of burning of the energetic materials (EM) again began to have extreme importance. For successful solution of problems, connected with suppression of the SPS combustion instability are necessary have detailed understanding about essence of mechanisms of the EM unstable burning on the new qualitative level. The experimental data independently obtained by various authors and for various kinds of evaporated EM shows the - on the burning surface are formed the existential cellular structures. This phenomenon was a subject of many investigations already more than four decades, however within the framework of the combustion classical theory the mechanism of its excitation and development does not find an adequate explanation. Detailed analysis and mutual comparison of investigations executed in this area and also detailed analysis of the experimental data, obtained in adjacent areas of science and engineering has allowed suggesting the new mechanism of occurrence of this phenomenon. This new concept connected, mainly, with excitation of the synergetic dissipative spatial-periodic micro-structures (SPMS) in the thin liquid-viscous layer and on the EM burning surface and determining the burning wave spatial instability. Obviously, it is possible to speak about the fundamental law determining the processes of the EM burning: the phenomenon of the SPMS formation has universal nature. On the EM burning surface occurs transition from the isotropic medium to the medium with existential structure. The process of the SPMS formation provides influence on the process of agglomeration and on the spectrum of agglomerates on the burning surface of heterogeneous EM. Within the scope of suggested concept, the physical-chemical effects taking place at erosive burning of the EM, receive a new explanation. On the basis of suggested concept the new technologies for suppression of combustion instability are developed. Application of suggested technologies in practical systems will allow control the development of physical- chemical processes at a new qualitative level.

NTREM, PARDUBICE, 2005 page 271-299

DECOMPOSITION KINETICS OF GAP BINDER IN THE PRESENCE OF AN ENERGETIC COMPONENT

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Abstract:

Glycidyl Azide Polymers (GAP) are promising candidates as energetic binders for future solid composite propellants. They produce minimum smoke, cause reduced pollution, and have low sensitivity. In our hands, we have undertaken a study of the decomposition kinetics of energetic binder in the presence of the energetic oxidizer, to assess the stability of the composite formulation.

We now report the decomposition kinetics of GAP binder in the presence of two high performance and environment friendly oxidizers like Ammonium Dinitramide (ADN) and4,10-dinitro-2,6,8,12-4,10-diazatetracyclo-[5.5.0.0^{5,9} 0^{3,1}1]dodecane (TEX). Thermal gravimetric analyses (TGA) and differential scanning calorimetry (DSC) were used to investigate the decomposition characteristics and heat of decomposition of TEX/GAP and ADN/GAP gum formulations. Addition of GAP has improved the thermal stabilities of both AND and TEX. GAP has been found to be more vulnerable to thermal decomposition in the presence of TEX than in the presence of ADN.

NTREM, PARDUBICE, 2005 page 300-305

DECOMPOSITION OF ENERGETIC MATERIALS INVESTIGATED BY MOLECULAR SIMULATIONS: HNIW, TNA

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Abstract:

Classical molecular dynamics simulations in Cerius^2 modelling environment were used to describe the decomposition process of crystal structure 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo [5.5.0.05,9.0^{3,11}] dodecane known as HNIW and 1-amino-2,4,6-trinitrobenzene, known as TNA. The dynamics simulations were carried out in 3D periodic systems of above mentioned crystal structures under high initial temperatures related to impact sensitivity. Dynamics trajectories were saved for a series of initial temperatures in the range 300 K -1000 Kfor HNIW and in the range 1000 K-5000 Kfor TNA. The detailed analysis of the dynamics trajectories allows us to describe the mechanism and kinetics of decomposition processes under selected high temperatures. Higher values of temperature decrease the calculation time corresponding to the rupture of the first N-NO_2 bond and also dramatically increase the kinetic energy of the system.

NTREM, PARDUBICE, 2005 page 306-315

THE PHASE STABILIZATION OF AMMONIUM NITRATE BY POTASSIUM DINITRAMIDE - A DIFFERENTIAL SCANNING CALORIMETRIC STUDY

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Abstract:
Ammonium nitrate (AN) has long been considered as a desirable oxidizer for solid rocket propellants and explosives because of its low cost, low sensitivity, low smoke signature and the absence of halogen atoms. The stumbling block for the application of AN as rocket propellant oxidizer is its dimensional instability caused by polymorphic transitions near the propellant processing and storage temperatures and its extreme hygroscopicity leading to unpredictable ballistic performance and catastrophic rocket motor failure. The phase transitions leading to volume change can be overcome by the use of phase stabilizers. Unfortunately most of the phase stabilizers used to prepare phase stabilized ammonium nitrate (PSAN) are non-energetic and the overall energy content of the formulation is reduced to a great extent. Therefore it is necessary to have PSAN with improved energy content. The present paper discusses the differential scanning calorimetry (DSC) study of potassium dinitramide (KDN)-AN compositions. Concentration levels ofKDN in the range of 0.2 to 5% (by weight) were studied. The results obtained show that at concentration levels above 3%, KDN has better phase stabilization effect on AN.
NTREM, PARDUBICE, 2005 page 316-323

MAMMALIAN CELL CYTOTOXICITY OF NITROAROMATIC EXPLOSIVES AND THEIR DEGRADATION PRODUCTS: THE ROLE OF OXIDATIVE STRESS

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Abstract:
Toxic effects of nitroaromatic explosives on mammalian species are attributed to their single-electron reduction by flavoenzymes (redox cycling of free radicals and oxidative stress), and/or to their two-electron reduction (formation of alkylating nitroso- or hydroxylamino products). In this work, we summarize the data on the enzymatic reactivity of explosives (2,4,6-trinitrotoluene (TNT) and its amino- and hydroxylamino- reduction products, tetryl, pentryl, tetranitrocarbazole, dinitrobenzofuroxan, nitrotriazoles, tetranitrobenzimidazolone) and model nitroaromatic compounds, and their cytotoxicity in bovine leukemia virus-transformed lamb kidney fibroblasts (line FLK). Cytotoxicity of compounds increased with an increase in their single-electron reduction potential (E^1 7) or their reactivity in enzymatic single-electron reduction reactions catalyzed by NADPH:cytochrome P-450 reductase or ferredoxin:$NADP^+$ reductase, and did not follow their reactivity in DT-diaphorase-catalyzed two-electron reduction. Further, the cytotoxicity was reduced by antioxidants, whereas dicumarol, an inhibitor for DT-diaphorase, showed minor and equivocal effects. It shows that the cytotoxicity of explosives in this cell line is caused mainly by the oxidative stress. The cytotoxicity of amino- and hydroxylamino-DNTs was lower than that of TNT, but higher than one may expect from their redox cycling activity. Thus, the additional modes of their cytotoxicity may be involved. Our data imply that the evaluation of redox properties of new explosives and high energy compounds in enzymatic systems may be a useful approach to characterize or predict their toxic properties.
NTREM, PARDUBICE, 2005 page 324-333

APPLICATION OF THE METHOD OF GRAY INTERRELATION ANALYZING TO ASSESS HAZARD OF GAS EXPLOSION ACCIDENTS

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Abstract:
Based on safety engineering science principle and local investigation, with an aim at situation of preventing gas, gas inherent hazard is put forward, and the gas gush quantity and gas pressure are inherent. The change of gas gush quantity in a period is nonlinear, gas inherent hazard is nonlinear and dynamic, the relation between gas inherent hazard and gas lure hazard is analyzed by nonlinear gray interrelation method. Furthermore, risk of gas hazard in roadway is analyzed with the gas gush quantity, the wind quantity and the gas concentration, it is significance on spot.
NTREM, PARDUBICE, 2005 page 334-339

DESIGN OF PARTICULATE ENERGETIC MATERIALS

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Abstract:
The crystal quality and the internal microstructure of crystals have a great influence on the sensitivity of energetic materials. Besides, the particle size and the particle size distribution are of great importance to the processing technology of energetic materials. Particle properties can especially be influenced by applying different crystallization techniques, such as cooling crystallization, membrane crystallization, emulsion crystallization and others.
The goal of the investigations was to determine the interrelationship between the properties of the gained crystals and the process parameters. Special attention was directed to the qualitative and quantitative examination of crystal defects and their dependence on the experimental conditions. Besides, the morphology and structure of crystals were calculated by molecular modelling. The effect of crystal defects on the sensitivity of the material was tested on different collectives of particles having varying amount of crystal defects.
NTREM, PARDUBICE, 2005 page 340-352

REGARDING THE DETERMINATION OF EXPONENT FROM BURNING RATE LAW OF POWDER, USING THE CLOSED BOMB DATA

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Abstract
In this paper it is presented a mathematical model of firing phenomenon from a ballistic system. In this model is used an expression for burning rate law of powder, in which the exponent has a variable value. This exponent is calculated using the curve of gases pressure versus time obtained at the burning of powder in closed 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 barrel and versus time. For an extant ballistic system, the theoretical results, obtained with the aid of this soft and the experimental data are compared.
NTREM, PARDUBICE, 2005 page 353-360

MAIN CHARGE INITIATION OF INSENSITIVE MUNITIONS BY "UNPLANNED STIMULI". FAST COOK-OFF RESISTANCE OF PRESSED PBX

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Abstract:
Energy transfer by shock, impact and heat are the basis for the initiation of warheads "on demand" as well as by "unplanned stimuli". Heat is involved in every kind of HE initiation and fire is a threat for a warhead which is always present, from the production over transportation and storage up to its use. So the thermal behaviour of an explosive is important for the Initiation of a PBX charge and the Cook-off safety of ammunitions. Moulding powder properties, heat transfer calculations and small scale tests help in the design of Fast Cook-off resistant press-filled warheads.
NTREM, PARDUBICE, 2005 page 361-369

FROM BINARY MIXTURES TO COMPLETE AMMUNITION COMPATIBILITY -A WHOLE CARTRIDGE IN ONE TAM AMPOULE-

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Abstract:
The determination of compatibility between explosives and contact materials in ammunition is an important test. It is mandatory while a final (type) qualification is performed. STANAG 4147 allows different methods to determine the compatibility which are able to demonstrate whether a reaction between explosives and other ammunition components occur or not. All tests require binary mixtures of explosive and contact material in a 50:50 ratio. This is said to be a worst case scenario, meaning that if no reaction is observed in a 50:50 mixture of minced materials then there will be no reaction in the real environment, where the mixture ratio is often like 95:5 and the materials consist of big pieces with a small surface to volume ratio. But binary mixtures do not consider the reality at all. One may think about reactions with three (or more) partners. For example, we have found out that in a 9 mm ammunition a reaction is going on between the solvent in the propellant with one component of the primer mixture which is catalyzed by the presence of copper. If only binary mixtures were checked then this reaction would have remained undetected. Therefore we have decided to measure complete ammunition in the microcalorimeter (TAM) to be sure to have followed all reactions that are going on in the cartridge. Unfortunately most ammunition articles are too big to be introduced into a 4 or 20 ml TAM ampoule. Therefore we had to simulate a complete cartridge by adding all components in a realistic weight or volume ratio in a TAM ampoule. The comparison of the microcalorimetry signal of these 'demonstrators' with the microcalorimetry signal of real ammunition shows whether this is a suitable way to go ahead or whether other parameters than mass, surface or volume ratio determine the microcalorimetry signal of the ammunition. We have tested two small calibre ammunition articles (a 9 mm cartridge and a 5.56 mm cartridge) by variation of their ingredients (propellant, metal, lacquer, primer). It could be shown that - besides the overall loading density - the ratio between propellant and primer is the main parameter to shift the microcalorimetry signal of this 'demonstrator' as close as possible into the pattern of the microcalorimetry signal of the complete cartridge.
NTREM, PARDUBICE, 2005 page 370-386

THE STUDY OF CHEMICAL MICRO-MECHANISM OF NITRAMINES INITIATION WITH UTILIZATION OF ^{15}N NMR CHEMICAL SHIFTS

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Abstract:
A brief survey is presented of the author's results obtained from studies of the chemical micro-mechanisms of nitramines initiation from the point of view of organic chemistry. The relationships have been presented and discussed between the characteristics of impact and electric spark sensitivities, detonation and thermal decomposition, on the one hand, and ^{15}N NMR chemical shifts of nitrogen atoms ofnitramino groups, on the other. In the case of the impact sensitivity, the said relationships involve the ^{15}N shifts of the amino nitrogen atoms carrying the nitro group primarily split off from the molecule. In the case of the initiation by shock, heat and electric spark, the ^{15}N shifts of nitrogen atoms in the primarily split off nitro groups themselves are involved. It has been stated that the chemical micro-mechanisms of primary fission processes of molecules of nitramines in the initiation by mechanical stimuli (inclusive the detonation course) and electric spark should be the same as in the case of their low-temperature thermal decomposition. Also mentioned is relevance of the modified Evans-Polanyi-Semenov relationship. On the basis of the findings presented it also has been stated that the detonation transformation itself of the nitramines should be preceded by an induction period.
NTREM, PARDUBICE, 2005 page 387-398

HIGHLY EXPLOSIVE NANOSILICON-BASED COMPOSITE MATERIALS

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Abstract:
We present a new composite energetic material based on nano-silicon. Two configurations of possible explosive systems can be realized. First, porous silicon (PSi) itself as explosive material in combination with common oxidizers and second, as enhancing additive to commonly used high explosives. Commonly, PSi has been produced from bulk Si wafers by electrochemical etching in an HF/ethanol mixture. This method is completely compatible with the standard silicon technology and full bulk silicon wafers can be processed to achieve the required explosive configuration. After filling the pores with oxidizer a 2D-explosive system can be realized. It reveals a variety of new possible applications in different industrial fields, e.g. as a novel, very fast airbag igniter. Unfortunately, this technique does not allow the production of large amounts of PSi and its costs are extremely high. Therefore, we developed a new concept of large scale production of PSi powder. It is based on "stain-etching" of commercially available polycrystalline bulk Si powder. This new technique expands further the variety of new possible applications of Si nanocrystals in energetic materials. In our presentation we will explain the preparation techniques and discuss the morphology and the physical properties of the resulting porous materials. Different parameters of the reaction were determined for several combinations of PSi and oxidizers by laboratory experiments. Among them are the time of chemical reactions, the reaction temperature, and the propagation speed of the shockwave. The energy yield was found to be as high as 9.2 kJ/g for a stoichiometric ratio of fuel (PSi) and oxidizer.Finally, we will also present the results of first experiments with PSi and fine polycrystalline Si powder as an enhancing additive to common high explosives. We will outline the advantages of the composite energetic materials containing nanosilicon, with respect to commonly used aluminum powder.
NTREM, PARDUBICE, 2005 page 399

THERMAL STABILITY OF THE IMPURITIES AND THE POLYMORPHS OF HNIW

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Abstract:
2,4,6,8,10,12-heksanitro-2,4,6,8,10,12-heksaazatetracyclo [5.5.0.0^{5,9}0^{3,1}1]dodecane (HNIW) is highly dense and one of most powerful explosive materials. Four polymorphs (α, β, γ and ε) have different molecular conformation, mechanical sensibility and thermal stability.
Phase transitions in the α-, β-, γ-, and ε-polymorphs ofHNIW have been studied as a function of temperature. High temperature equilibrium solvation studies coupled with Fourier transform infrared spectroscopy (FTIR) for the identification of polymorphic conversion indicated a thermodynamic stability order of ε> γ> α-hydrate > β, with the epsilon polymorph the most thermodynamically stable phase ofHNIW. These results are agreement with data from Differential Scanning Calorimetry (DSC). The thermal stability is also related with purity of energetic materials. 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo[5.5.0.0^{5,9}0^{3,11}] dodecane (TEX) and 2-acetyl-4,6,8,10,12-pentanitro-2,4,6,8,10,12-heksaazatetracyclo[5.5.0.05^{,9}0^{3,11}]dodecane are two main separated and identified impurities. Both these impurities are more thermodynamically stable than HNIW. Differential Scanning Calorimetry (DSC) studies showed impure HNIW to be more thermodynamically stable then pure 2,4,6,8,10,12-heksanitro-2,4,6,8,10,12-heksaazatetracyclo[5.5.0.0^{5,9}0^{3,11}]dodecane.
NTREM, PARDUBICE, 2005 page 400

DETONATIVE IGNITION OF METAL/FLUOROCARBON PYROLANTS

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Abstract:
Fuel rich metal/fluorocarbon pyrolants play an important role as either infrared decoy flare materials orpropellant igniters [1]. Recently the viability of metal/fluorocarbon pyrolants as reactive fragments for enhanced blast effects has been studied in the US [2]. In addition the behaviour of Magnesium/Teflon/Viton payloads in common IR decoy flares is now investigated in several countries with respect to sensitivity towards bullet impact and close detonation of warheads. So far there have been only reports about mechanical shock ignition of pyrotechnics and propellants with accelerated thin films [3]. We report in this paper about the detonative ignition of a series of consolidated metal fluorocarbon pyrolants in close contact to high explosives. Upon subjection to a shock wave metal fluorocarbon pyrolants ignite. The paper discusses the ignition mechanism and propagation aspects of the reaction. A series of metal fluorocarbon mixtures based on either magnesium, aluminium and titanium as well as polytetrafluoroethylene and graphite fluoride are investigated.
NTREM, PARDUBICE, 2005 page 401

INVESTIGATION OF DEFLAGRATION TO DETONATION TRANSITION IN POROUS HIGH EXPLOSIVE BY SYNCHROTRON RADIATION APPROACH

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Abstract:

We present facility of new experimental approach for physics explosion. Contemporary electron accelerator can produce roentgen radiation (synchrotron radiation) with features that are very attractive for experimental physics at all and for explosion physics especially. In present paper we discuss one method for detecting density dynamics by synchrotron radiation.

The main idea of method is next. We can radiograph investigated charge of explosive by synchrotron radiation beam and detect weakened radiation intensity. Use this information and appropriate calibration we can restore amount of radiograph matter. At present we can use radiation beam with "knife" shape: thickness 0.1 mm and width 15 mm. Gas line detector, which measure weakened radiation intensity, has 256 space strips with 0.1 mm interval and memory for 32 frames, with time between frames 0.5 mks. As a result of one experiment we have "slit roentgen cinema" of explosion process. Such high space and time resolution are very attractive for explosion detecting. As a one result of method we present some new experimental data for deflagration to detonation transition in charges of porous hay explosive (petn, rdx), with density near 1 g/cm^3. In experiment we measure weakening of transmitted beam through bit core of investigated charge. We can obtain compression dynamic ρdl versus time and space duration along charge axes. As a result in one experiment we obtain all density dynamic for deflagration to detonation process, from initiation moment to stationary detonation wave.

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INSENSITIVE INITIATION CHAINS FOR INSENSITIVE EXPLOSIVE FILLS

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Abstract:

Based on the work on insensitive high explosive mixtures presented on the G.-Int. Seminar and other high explosive materials we are developing insensitive initiation chains for existing sensitive fuze systems and new designs to fully meet the existing MIL Std 2105 B and the follow on STANAG 4439. During presentation technical related issues deducted from the high explosive main fillings required by the given threat requirements consequences on the components of initiation chains will be discussed and some of the existing technical solutions presented.

NTREM, PARDUBICE, 2005 page 403

STRUCTURE-KINETIC LAWS OF THERMAL DECOMPOSITION OF SIX-MEMBERED CYCLIC N-NITRAMINES

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Abstract:
The thermal decomposition of six-membered cyclic N-nitramines, contained in ring one, two and three nitramine fragments, and also oxy-, gem-dinitro, azido and tetrazole function, is investigated, using manometer method combined with chromatography, FTIR-spectroscopy and mass-spectrometry. Influence of functional groups on the rate and activation parameters of N-nitramines decomposition limited stage is established.
NTREM, PARDUBICE, 2005 page 404

MASS SPECTROMETRIC ANALYSIS OF NOVEL NITRAMINE EXPLOSIVES - HNIW AND DTIW

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Abstract
The current paper describes the development of mass spectrometric methods for the analysis of two novel nitramine explosives - Hexanitrohexaazaisowurzitane (HNIW) and 4,10-Dinitro-2,6,8,12-Tetraoxa-4,10-Diazaisowurzitane (DTIW). The methods include electrospray (ESI) and atmospheric pressure chemical ionization (APCI) techniques for liquid chromatography mass spectrometry (LC/MS), chemical ionization for direct introduction (DCI) and gas chromatography mass spectrometry (CI-GC/MS). It is found that HNIW (438 Da) is detectable using both positive and negative modes of DCI and in the negative mode, using ESI in combination with LC/MS. Several anions were found to complex with HNIW, e.g. CF_3CO_2-, Cl-, Br-, I-, NO_3- and NO_2-. On the other hand, DTIW could only be detected using positive DCI and CI-GC/MS, where an MH+ ion (m/z 263) was formed. An interesting loss of an oxygen atom was observed ($[MH-1\ 7]^+$, m/z 246) in the iBuCI mass spectra of DTIW, which could be explained by the loss of iBuOH from the $[M+57]^+$ attachment ion. The fragmentation pathways of the two nitramines were further studied by MS^2 experiments. It was found that the main fragmentation pathway of the MH+ ion of DTIW involves the loss of nitrous acid (HNO2). The fragmentations of anion adducts of HNIW were studied using both CID (using an FTICR and an Ion Trap) andIRMPD (with an FTICR). Several anion adducts gave rise to [438 Da + anion]$^-$ ions, which fragmented back to the neutral HNIW and the added anions. However, Cl-, Br-, NO3- and NO_2– afforded a series of fragments that resulted from the isowurzitane structure. It was found that under more energetic conditions (e.g. IRMPD and high pressure CID) more informative CID spectra are produced. It is also apparent that the attached anion affects the course of fragmentation. Thus Ion trap CID MS^2 experiment of the Br- adduct produced the "poorest" spectrum with one fragment ion at m/z 371 (for ^{79}Br), attributed to the loss of $C2H_2$[NNO2] 2, while the corresponding $[M+Cl]^-$ and $[M+NO2]^-$ ions gave rise to HNO2 losses together with the consecutive loss of$C2H_2$[NNO2]2. Hence the CID spectrum of the $[M+Br]^-$ ion was found to be the best suited for analytical purposes. In order to understand some of the HNIW fragmentation pathways, theoretical calculations are being used.
NTREM, PARDUBICE, 2005 page 405

VACUUM STABILITY TEST (VST) – CALIBRATION AND COMPARISON OF MERCURY AND PRESSURE TRANSDUCER METHODS

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Abstract:
VST is the most fundamental method used to assess thermal stability and compatibility of energetic materials. The volume of gas evolved upon heating under vacuum is measured and according to the amount of gas a material is declared stable, or a mixture compatible. This paper compares mercury manometer VST and pressure transducer VST.
The traditional method of measuring the volume of evolved gas is using a mercury manometer (VSTHg). The desire to eliminate the extensive use of mercury motivated the development of an electronic version using pressure transducers (VSTPT). Both VSTHg and VSTPT have been accepted as NATO standards (STANAG 4556 and STANAG 4147).
Comparison between the two methods is essential before abandoning the traditional mercury base method. For this purpose a unique calibration method was developed. It is based on a reaction which evolves a predictable amount of gas in the temperature range of the test. A mixture of a solid acid which melts in the 90°C-120°C range and only then reacts with a metal carbonate releasing a predicable amount of carbon dioxide was looked for. Based on melting points, glutaric acid was chosen. When melted, the diacid reacts quantitatively with a simple carbonate, giving carbon dioxide according to the following reaction: M_2CO_3 (s) + 2RCOOH (s) + 2RCOOM (s) + H_2O (l) + CO_2 (g) Where M = K or Na.
The volume of CO2 evolved is stochiometrically proportional to the salt weight and only carbon dioxide remains as a gas at room temperature, hence the amount of gas could be calculated theoretically. The results obtained from VSTHg and VSTPT were almost identical and are in excellent agreement with theoretical values. Hence the calibration method is quantitative, reproducible and may be applied on both VSTHg and VSTPT methods.In addition, test results from VSTHg and VSTPT of a series of 18 mixtures (energetic and nonenergetic) were compared. A standard deviation of 7.3% ± 5.8% between VSTHg and VSTPT was obtained. Therefore the two methods are interchangeable and the VSTPT method was adopted for stability evaluation.
NTREM, PARDUBICE, 2005 page 406

DEVELOPING AND MAINTAINING SKILLS IN THE EXPLOSIVES SECTOR

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Abstract:
The manufacture and use of explosives, propellants and pyrotechnics underpins a significant part of the European Union economic and industrial activity. An understanding of explosives science and technology and the competence to harness it is central to maintaining European Explosives capability, national security, and in sustaining a competitive European industry. There is a perception and some evidence that in Europe, competence level in this key technological area is being eroded. In several member nations a high proportion of the most experienced and knowledgeable personnel are retiring or nearing retirement. Urgent efforts are therefore underway in some partner nations to replenish this expertise. The UK together with Sweden, Norway, Finland and Italy are taking part in a Leonardo Da Vinci programme to develop a comprehensive framework which describes and categories all of the competences of workers engaged in the manufacture or use of explosives. This paper will outline i) the procedures used to develop the competences for UK workers and ii) the development of National Occupational Standards for the UK and Europe.
***NTREM, PARDUBICE, 2005 page* 407**

NUMERICAL SIMULATIONS OF OIL-WELL PERFORATOR USING 3D LAGRANGIAN LS-DYNA CODE

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Abstract:

Fast dynamics of an oil-well perforator was numerically simulated by using 3D Lagrangian LS-DYNA code covering explosive detonation, liner collapse and jet formation. In the analysis, the influence of liner mesh density on jet parameters was studied. It was demonstrated that for a perforator analysed, the liner had to be divided into around ten elements across the liner thickness. The analysis showed that 3D explicit LS-DYNA is still an efficient and useful numerical tool for prediction of shaped charge jets formation, in spite of current effort that is focused on ALE numerical techniques in thisfield.

NTREM, PARDUBICE, 2005 page 408-414

PARAMETERS OF HEAT EXPLOSION AND DETONATION OF HEXANITROMANNITE AND NITROTHREEAZOLONE

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Abstract:

The main goal of investigation was to compare the explosion parameters of essentially different explosives: hexanitromannite (HNM) and nitrothreeazolone (NTO). HNM is a nitroester, and NTO is insensitive explosive. Explosion hazard of liquid nitoesters supposes to be very high, failure detonation diameter of them is very low (df ~ 2 mm for nitroglycerine and nitroglycole), and character oh heat explosion of them is very intensive. HNM is solid substance, and its detonability was investigated for charges in cast state and for a solutions of HNM in liquid nitroglycole. The dependence of df of nitroglycole vs. initial temperature was used for estimation df of HNM in molten state. The estimation gave a value of critical diameter df = 0.7 mm at t = 120 0C. At d = 1.3 mm in long glass capillary low velocity detonation was registered in cast charge of HNM, at diameter d = 2.2 mm in such charge high velocity detonation propagated. Detonation velocity of pressed NTO was measured in steel tubes at density = 1.48 g/sm3, D = 6.34 – 6.38 km/s. The dependencies of heat explosion delay vs. initial temperature was measured for both substances. Their kinetic parameters were calculated using these dependencies.

NTREM, PARDUBICE, 2005 page 415-421

COMPARISION OF EXPLOSIVE PARAMETERS OF PEROXIDES AND OF NITROCOMPOUNDS

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Abstract:
The ultimate objectives of investigation were benzoyl peroxide and cumene hydroperoxide. We carried out the experiments with above named peroxides and with typical explosive (TNT, PETN and NTO) for comparison applying method of Differential Scanning Calorimeter. The method does not permit to measure the heat of decomposition of the reactions which are accompanied with gas formation. Comparison of dependencies of heat flux vs.temperature of benzoyl peroxide decomposition and of TNT, NTO and even of PENT visually demonstrates that decomposition of peroxide begins at fusion, and nitrocompounds decompose at rather higher temperature than its melting point. High explosion hazard of benzoyl peroxide is explained by low temperature of decomposition, high intensity of heat explosion and high ability and high burning velocity.
***NTREM, PARDUBICE, 2005 page* 422-429**

2-NITRIMINO-5-NITROHEXAHYDRO-1,3,5-TRIAZINE: STRUCTURE AND PROPERTIES

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Abstract:
The 2-nitrimino-5-nitrohexahydro-1,3,5-triazine (NNHT) structure was solved by methods of X-ray analysis. Kinetics of a thermal decomposition was investigated under isothermal conditions by manometric method in solid phase and solution. The decomposition products were investigated by mass-spectrometric method. The impact sensitivity of NNHT was investigated with the help of fallhammer test. The sensitivity to explosion by heat was determined as the temperature of flash and time to explosion delay. Energetic and detonation parameters of NNHT were estimated using thermodynamic method with BKW equation of state and by simple correlation methods.
NTREM, PARDUBICE, 2005 page 430-443

REACTIVITY OF 2-(DINITROMETHYLENE)-4,6-DIHYDROXY-5,5-DINITROPYRIMIDINE IN THE PROCESSES OF NUCLEOPHILIC SUBSTITUTION

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Abstract:
The main routes of transformations of 2-(dinitromethylene)-4,6-dihydroxy-5,5-dinitropyrimidine in reactions with primary aliphatic amines, ammonia, hydrazine and its derivatives in aqueous solution are considered and the mechanism of the processes is suggested. The formation of derivatives of 2-dinitromethyl-5-N-alkyl substituted 1,3,5-triazines and 3-dinitromethyl-1,2,4-triazolone is demonstrated.
NTREM, PARDUBICE, 2005 page 444-450

STUDIES ON THE HYDRODENITRATION BY TIN (II) CHLORIDE OF POLYNITROHEXAAZAISOWURTZITANES

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Abstract:
The hydrodenitration of 2,4,6,8,10,12-hexanitro- (HNIW, CL-20), 2,4,6,8,12-pentanitro- and 2,6,8,12-tetranitro-hexazaisowurtzitane using SnCl2 has been studied. Removal of N-nitro groups from HNIW to give the two isomeric mono-amines occurs with almost statistical distribution of products, but hydrodenitration of 2,4,6,8,12-pentanitrohexaazaisowurtzitane more strongly favours reaction at the nitramine groups in the 5-membered rings. Surprisingly, reduction of the di-amine 2,6,8,12-tetranitrohexaazaisowurtzitane did not give the expected tri-amine 2,6,8-trinitrohexaazaisowurtzitane but the ring-cleavage product 1,1,2,2-tetranitraminoethane instead.
NTREM, PARDUBICE, 2005 page 451-458

SYNTHESIS AND PROPERTIES OF SALTS OF 3,5-DIAMINOPICRIC ACID

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Abstract:
Seven salts of 3,5-diaminopicric acid, ammonium 3,5-diaminopicrate (ADAP), hydrazinium 3,5-diaminopicrate (HDAP), guanidinium 3,5-diaminopicrate (GDAP), aminoguanidinium 3,5-diaminopicrate (AGDAP), diaminoguanidinium 3,5-diaminopicrate (DAGDAP), triaminoguanidinium 3,5-diaminopicrate (TAGDAP) and guanylurea 3,5-diaminopicrate (GUDAP) have been synthesized [from 3,5-diaminopicric acid (DAPA) and the corresponding base (or its salt)] and characterized by 1H, 13C, and 15N NMR spectroscopy, FTIR, DSC, TG, SEM and CHN elemental analysis. Their heats of combustion were measured by bomb calorimetry and their heats of formation calculated. Their impact sensitivities were also measured. Some of these salts (GDAP, AGDAP and GUDAP) are extremely insensitive to impact (F of I > 130), whilst others (HDAP and TAGDAP) might be useful as initiators (F of I . 30).
NTREM, PARDUBICE, 2005 page 459-464

THE USE OF THE TRIFLUOROACETYL GROUP TO PROTECT NH AND OH GROUPS DURING NITROLYSIS REACTIONS

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Abstract:
N and O trifluoroacetylation has been used to protect secondary amine groups and hydroxyl groups respectively during nitrolysis reactions. The trifluoroacetyl group may be readily removed from the energetic products by solvolysis under mild conditions. Examples include the synthesis of 2,4,6,8,12-pentanitrohexaazaisowurtzitane, 2,6,8,12-tetranitrohexaazaisowurtzitane, 2,2-bis(nitratomethyl)propan-1-ol and N-nitroazetidin-3-ol.
NTREM, PARDUBICE, 2005 page 465-471

TLC ANALYSIS OF DADNE AND SOME INTERMEDIATE PRODUCTS OF ITS SYNTHESIS

Jan Błądek, Sylwia Pietrzyk, Stanisław Cudziło, and Zbigniew Chyłek
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Abstract:
In the paper, results of research on application of thin layer chromatography (TLC) for determination of 1,1-diamino-2,2-dinitoethene (DADNE) and its precursors produced in the synthetic path starting from 2-methylpyrimidine-4,6(3H,5H)-dione. Analytical parameters of the substances and methodology of their quantitative analysis were determined, and the results obtained were used for controlling the DADNE synthesis process.
NTREM, PARDUBICE, 2005 page 472-476

DETERMINATION OF POST-EXPLOSION RESIDUES OF AMMONIUM NITRATE IN ENVIRONMENTAL SAMPLES

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Abstract:
The paper presents results of determination of ammonium nitrate, which remains in detonation products of industrial explosives. Charges of the explosives containing ammonium nitrate were detonated inside samples of concrete, sand and wood. After detonation, we tried to detect ammonium nitrate in the matrixes using instrumental thin layer chromatography (TLC). In this way a possibility of identification and determination of ammonium nitrate on the spot of criminal events was confirmed.

INTERACTIONS BETWEEN THE NITRAMINES RDX, HMX AND CL20 WITH THE ENERGETIC BINDER GAP

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*** Department of Chemistry, University of Edinburgh, Edinburgh, U.K.

Abstract:
The nitramines RDX, HMX and Cl-20 are commercially used as explosives. We investigated their decomposition pathways computationally and modelled their decomposition in the presence of the energetic binder GAP.
NTREM, PARDUBICE, 2005 page 477-484

THE INFLUENCE OF PHYSICAL STRUCTURE OF AMMONIUM NITRATE PRILLS ON DETONATION PROPERTIES OF ANFO-EXPLOSIVES

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Abstract:

A structure of ammonium nitrate prills about different porosity has been examined by using scanning electron microscope. Porous prills have been obtained from agricultural product by thermal treatment. Detonation velocity and cylinder expansion test have been run for ANFO made from above-mentioned prills. Disclosed by microscopic examinations prills' structures have been related with detonation properties of ANFO manufactured from different kind of prills.

NTREM, PARDUBICE, 2005 page 485-494

DETONATION ARRESTER PERFORMANCE FOR HYDROGEN-AIR MIXTURES

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Abstract:

Experimental data on the feasibility of a specific detonation arrester are provided in this study. This new type of arrester consists in a series of segments filled with shot. The data are aimed at demonstrating the pertinent use of this type of arrester for the safety in the chemical and oil industry. The experimental results show that this device is appropriate for quenching of flame and detonation in hydrogen-air mixtures.

NTREM, PARDUBICE, 2005 page 495-499

IMPROVED SYNTHESIS AND X-RAY STRUCTURE OF 5-AMINOTETRAZOLIUM NITRATE

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Abstract:

5-Aminotetrazolium nitrate was synthesized in high yield and characterized using Raman and multinuclear NMR spectroscopy (1H, 13C, 15N). The molecular structure of 5-aminotetrazolium nitrate in the crystalline state was determined by X-ray crystallography: monoclinic, P 21/c, a = 10.5493(8), b = 3.4556(4), c = 14.606(1) A, ß = 90.548(9)°, V = 532.44(8) A3, Z = 4, . = 1.847 g cm-1, R1 = 0.034, wR2 (all data) = 0.090. The thermal stability of 5-aminotetrazolium nitrate was determined using differential scanning calorimetry, the compound decomposes at 169°C. The enthalpy of combustion (.Hcomb.) of 5-aminotetrazolium nitrate ([CH4N5]+[NO3]-) was determined experimentally using oxygen bomb calorimetry: .Hcomb.([CH4N5]+[NO3]-) = -6020 ± 200 kJ kg-1. The standard enthalpy of formation (.H°f) of [CH4N5]+[NO3]-was obtained on the basis of quantum chemical computations at the electron-correlated ab initio MP2 (second order Moller-Plesset perturbation theory) level of theory using a correlation consistent double-zeta basis set (cc-pV-DZ): .H°f([CH4N5]+[NO3]-(s)) = + 87 kJ mol-1 = + 586 kJ kg-1. The detonation velocity (D) and the detonation pressure (P) of 5-aminotetrazolium nitrate was calculated using the empirical equations by Kamlet and Jacobs: D([CH4N5]+[NO3]-) = 8.90 mm µs-1 and P([CH4N5]+[NO3]-) = 35.7 GPa.

NTREM, PARDUBICE, 2005 page 500-509

MEASUREMENT IN BLAST HOLE STEM AND INFLUENCE OF STEMMING MATERIAL ON BLASTING QUALITY

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Abstract:

Paper presents results of blast hole stemm materials, that were conducted to assert best stemm materials for surface blasting in quarry of technical / construction stone. Blasting has been performed with equal explosives and test-minefield parameters (length of the stem, volume of the explosive charge, mine-drill depth, and angle) on various sites / quarry. Results are guidelines in materials to be chosen in surface blasting of quarry works, adding to quality of mining works and reduction of costs.

NTREM, PARDUBICE, 2005 page 510-519

MEASUREMENT OF SHOCK WAVE FORCE IN SHOCK TUBE WITH INDIRECT METHODS

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Abstract:
Explosives Lab of Mining Geological & Oil Faculty in Zagreb University is performing testing with aim of design of detonator that would unify advantages of non-electric system and precision in regulating interval in electric system. Sum of energy released by wave force in shock tube is a condition for work of this new detonator, and measurement of wave force is first step in determining of sum of energy. Sum of energy is measured indirectly, on two principles: movement sensors and strain gauges sensors.

NTREM, PARDUBICE, 2005 page 520-527

CHARACTERISTICS OF EXPLOSION-SAFETY OF AIR-METAL DUST SUSPENSIONS

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Abstract:
Ignition and burning of particulate metals was a subject of many investigations during for about half-of-a-century. Within the framework of the problem of this paper the modern state of the theory of ignition of metal particles in a hot oxidizing gas is described. The theory of ignition was developed on the base of the overall heat explosion theory of Semenov - Frank-Kamenetsky. Theory of burning of a particle was elaborated based, first, on the burning theory of a droplet of a liquid fuel and then it was modified with taking into account natural complications accompanying a metal particle oxidation. Experimental results that satisfy to the theories can be easily found among the numerous experimental data till now produced and it is the obvious success of the theory. The main goal of this paper is summarizing of literature experimental results in the light of modern scientific ideas.

NTREM, PARDUBICE, 2005 page 528-536

CRYSTAL STRUCTURES OF THE SILVER AND POTASSIUM SALTS OF NITROFORM

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Abstract:
Silver and potassium nitroformate were synthesized and the crystal structures were obtained.

NTREM, PARDUBICE, 2005 page 537-538

STUDY ON SAFETY OF EXPANDED AMMONIUM NITRATE EXPLOSIVE

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Abstract:
The safety properties of expanded ammonium nitrate(AN) explosive and its main composition were tested, such as the mechanical sensitivity, the sensitivity to auget, the sensitivity to shock wave and the sensitivity to spark of static electricity. The results show that the safety of expanded AN and expanded AN explosive is similar to that of common AN and its TNT-explosive.
NTREM, PARDUBICE, 2005 page 539-544

DETERMINATION OF METAL OXIDES AND THEIR CONCENTRATION IN THE IDENTIFICATION PARTICLES

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Abstract:
Identification Particles used for the purpose of the post blast identification of explosives, have a coding system based on the combination of metal oxides and their different concentration. These materials are consisted of the polymeric matrix, iron powder (ferromagnetic properties), UV light active dyestuff and various metal oxides in different ratio. A suitable analytical method must be applied for an accurate characterization of these metals components in the particles for finding needed information, it means to determine the production place, year of production and eventually production batch of misusing explosives. The flame atomic absorption spectrometry (F-AAS) performs rapid and sufficiently sensitive method suitable for this purchase. In this work, the method for the determination of ratio of oxides in a few types of identification particles using F-AAS is described. The microwave digestion was applied for the samples containing polybutadiene matrix, leaching with nitrohydrochloric acid was used if the samples have contained epoxide matrix. Using the described procedure, the determination was free of interferences so that a simple calibration curve method could be applied. The detection limits (LODs) for individual elements (lead, copper, magnesium and zinc) were 0.53 mg.l-1, 0.11 mg.l-1, 0.01 mg.l-1 and 0.11 mg.l-1, respectively.
NTREM, PARDUBICE, 2005 page 545-548

RESEARCH OF ARTIFICIAL AGEING SUITABLE CONDITIONS DURING THE INVESTIGATION OF PROPELLANTS LIFETIME

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Abstract:
This paper describes the investigation of the effect of different artificial ageing conditions on chemical stability of propellants. The chemical life of two samples of propellant was calculated by the depletion of stabilizer. The ageing conditions were choosing according to first study draft of AOP-48 edition 2.
NTREM, PARDUBICE, 2005 page 549-565

IMPROVED SYNTHESIS OF 2-(DINITROMETHYLENE)-4,5-IMIDAZOLIDINEDIONE

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Abstract:

Acetamidine sulphate and acetamidine hydrogensulphate were prepared from acetamidine hydrochloride by two different methods. Both acetamidine sulphate and hydrogensulphate were used for condensation reaction with diethyloxalate to produce 2-methoxy-2-methyl-4,5-imidazolidinedione, which was subsequently nitrated to 2-(dinitromethylene)-4,5-imidazolidinedione. The use of the mentioned acetamidines is convenient, since Soxhlet extraction can be removed from the reaction process and the yield is higher than in the case of acetamidine hydrochloride.

NTREM, PARDUBICE, 2005 page 566-570

ANALYSIS OF NITROAROMATIC COMPOUNDS IN SOIL ENVIRONMENTS

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Abstract:

Polynitro organic explosives are typical labile environmental pollutants that can biotransform with soil indigenous micro-organisms, photodegrade by sunlight and migrate through subsurface to groundwater contamination. To be able to determine nitroaromatic compounds and their (bio)transformation products in soil, a comprehensive analytical methodology of sample preparation, separation and detection is required. At first were taken different soil samples contaminated with nitroaromatic compounds and then they were analysed. Modern extraction techniques were tested for the determination – pressurised fluid extraction (PFE), supercritical fluid extraction (SFE) and ultrasonic extraction. Gas chromatography with mass detection (GC-MS) was used for the separation and detection.

NTREM, PARDUBICE, 2005 page 571-574

PROPERTIES OF A HIGHLY FRICTION SENSITIVE DERIVATIVE OF 1,5-DIAMINO-1H-TETRAZOLE (DAT): 1,5-DIAMINO-4-METHYLTETRAZOLIUM DINITRAMIDE

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Abstract:

The reaction of 1,5-diamino-1H-tetrazole (1) with iodomethane followed by the methathesis of the iodide (2) with silver dinitramide yields the highly friction sensitive 1,5-diamino-4-methyl-1H-tetrazolium dinitramide (3). 3 crystallize in the orthorhombic space groups P212121 and shows an intriguing interaction of one nitro group of the dinitramide anion with the tetrazolium cation. Preliminary sensitivity testing of the crystalline compound 3 indicates rather low impact sensitivity with a value of 7 J in contrast to the relatively high friction sensitivity of 24 N. The thermal decomposition of 3 was investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Mass spectrometry and IR spectroscopy were used to identify the gaseous decomposition products.

NTREM, PARDUBICE, 2005 page 575-584

DEVELOPMENT OF TESTING METHOD FOR DETERMINATION INITIATION STRENGTH OF DETONATORS BY MEASUREMENT IN IMPULSE CHAMBER

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Abstract:

A new testing method for determination of initiation strength of detonators is described. Results of some experimental investigations of measurement of explosion of detonators in impulse chamber are presented. The principle, mathematical apparatus and instrumental equipment of this new non-direct testing method are described. The method seems to be simple, prompt, with little demands for staff and measuring installation, economically practicable and safe, and could be used as a standard testing method for commercial detonators.

NTREM, PARDUBICE, 2005 page 585-594

PROPAGATION OF DETONATION IN CYLINDRICAL LOW-SENSITIVE HE SAMPLES

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Abstract:

The electrocontact and photochronographic procedures were used to study detonation propagation in cylindrical samples of different diameter made of insensitive HE for the cases of single-point and plane-wave initiation. The diameter of samples ranged from 15 to 120mm. The stationary detonation rate vs diameter of the cylindrical sample was constructed. The relation between the curvature of the detonation front and its rate is identified.

NTREM, PARDUBICE, 2005 page 595-599

THE SPIN-PULSATING REGIME OF DETONATION IN SOLID AND LIQUID EXPLOSIVES

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Abstract:
The work concerns to investigation of quite distinct inhomogenity in the detonation front in cast and liquid high explosives.. The experimental methodology of simultaneous registration of luminosity at detonation of cast charges on a base of TNT near charge surface and deformation of witnessplate are described. Experiments with ballistite propellant NB were carried out, and spin pulsation at detonation were observed too. Solutions of DNT in nitroglycole (NGL) were investigated with respect to possibility of spin detonation propagation. Results of investigation justify the conclusion of previous work that the necessary properties for low frequency spin detonation propagation are: detonation velocity of system must be D = 7.3-7.4 km/s and heat of explosion QV = 5.4 MJ/kg.
NTREM, PARDUBICE, 2005 page 600-606

INTRODUCTION TO THERMAL STABILITY STUDIES OF NITROBENZENE AND NITROPHENOL DERIVATIVES IN SULFURIC ACID

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Abstract:
Differential thermal analysis was used for evaluation of thermal stability of nitroaromatic byproducts from industrial manufacture of nitrobenzene. Influence of 70% sulfuric acid and traces of Fe2O3 on thermal stability of these byproducts was investigated for initial characterisation of risks of runaway reactions in waste liquids. It was found that 2-nitrophenol forms thermally unstable mixture with sulfuric acid and can thus act as a initiator of runaway reactions. As the only one from tested substances, it showed exothermal decomposition at temperatures below 100 oC. Presence of Fe2O3 in reaction mixtures at the applied experimental conditions does not influence onsets of exothermal decomposition reactions but changes their mechanisms.
NTREM, PARDUBICE, 2005 page 607-612

COMPARISON OF SMOKELESS NITROCELLULOSE POWDER PRODUCTION ACCIDENTS IN EXPLOSIA WITH THE WORLD'S ACCIDENTS DATABASE

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Abstract:
Smokeless nitrocellulose powder production technology is one of the most dangerous technologies in the chemical industry, because all chemicals used in high amount (without water) can be considered as explosives. Smokeless powder production in Explosia has begun in year 1924. Several causes from this year to present, defined as accidents, occurred. Therefore this contribution is focused on statistical evaluation of accidents in Explosia. Typical notes of these accidents are compared with world's accidents database for the same time period.
NTREM, PARDUBICE, 2005 page 613-622

EFFECTIVE AMMUNITION 20x102

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Abstract:
Within the framework of arming the Czech Army with weapon system "PL20", the requirement has been raised for development of effective ammunition for firing on armored targets. This ammunition should serve at both weapon systems used at combat fighters, and for carriage weapon systems for land fire.
NTREM, PARDUBICE, 2005 page 623-631

SOME DETONATION CHARACTERISTICS OF AMMONIUM NITRATE-ALUMINUM-DOUBLE BASE PROPELLANT MIXTURES

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Abstract:
The influence of double base propellants (DBP) on detonation characteristics of ammonium nitrate-aluminium mixtures was assessed. Investigated explosive mixtures contained 20 and 40% of the propellants. We determined velocity of detonation, comparative strength and intensity of blast waves (peak blast overpressures) generated by the explosion of the mixtures. Positive phase impulses were also calculated. Some parameters of the compositions increased along with the propellant content.
NTREM, PARDUBICE, 2005 page 632-638

INACTIVE MODIFICATION OF AMMONIUM NITRATE AND THE DETERMINATION OF ITS ACTIVITY AS OXIDIZER IN EXPLOSIVES

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Abstract:
In China, in order to guard against terrifying activities by the explosive made from ammonium nitrate, Chinese government prescribes that agriculture ammonium nitrate is not allowed to put in market before it is modified so well that explosive can not be made from it through simple mixing. The method of modification is changing ammonium nitrate to compound fertilizer by adding calcium carbonate, urea, ammonium sulfate, etc. A testing method similar to UN cap sensitivity test was established primarily to assess the modification. Based on the content of ammonium nitrate in modified compound, diesel oil and wooden powder are mixed into it homogeneously by the proportion of ammonium nitrate/diesel oil/wooden powder=92%/2%/6%. The mixture is restricted in an iron tube(. 80mm×160mm×1mm) then initiated by 8th instantaneous electric detonator. A witness and steel base plate with thickness of 1mm as verifying plate is put underside the tube to estimate whether the detonation is complete.
NTREM, PARDUBICE, 2005 page 639-642

EFFICIENCY OF APPARATUS FOR TESTING SENSITIVITY OF EM TO ELECTROSTATIC DISCHARGE

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Abstract:
Expert literature describes various apparatuses for testing sensitivity of energetic materials (EM) to effects of electrostatic discharge. Besides, also various methodological and interpretation procedures have been extensively or in secondary issues introduced, which hinders comparisons of sensitivity of comparable EM. For instance, Kirshenbaum [1] gathered available data of initiation energies of discharge for Lead Azide RD1333, which vary in the interval from 4.10–10 to 2.10–2 Joule. This contribution presents besides the analysis of efficiency of the test circuit working in Short (oscillation) regime also several rules obeyed in the methodology of testing of a wide varied of EM by means of ESZ apparatus at DTTX. The paper has been written with the aim to contribute to more extensive standardisation of sensitivity tests of various EM by means of condenser pulse devices.
NTREM, PARDUBICE, 2005 page 643-651

DEVELOPMENT OF INSENSITIVE HIGH EXPLOSIVES – NITROGUANIDINE

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Abstract:
In the paper an insensitive high explosive nitroguanidine (NQ) is investigated. Obtaining technology of nitroguanidine is described and investigation of its explosive properties is carried out. Methods of NQ crystallization from various solvents are described. Spherical forms of NQ crystals were obtained, grain morphology dissolution, bulk density and tap bulk density were determined Differential thermal patterns are determined and spectrum in infra-red radiation is investigated. Density of obtained NQ, sensitivity to friction and impact were inspected. Mixtures of crystalline forms of NQ with high energy explosives (HE) such as hexogene (RDX) and oktogene (HMX) were prepared. The detonation velocity for selected mixtures was determined.
NTREM, PARDUBICE, 2005 page 652-662

APPLICATION OF TIME-TEMPERATURE SUPERPOSITION PRINCIPLES TO PREDICTION OF MECHANICAL PROPERTIES OF DOUBLE BASED ROCKET PROPELLANTS

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Abstract:
Because of their viscoelastic nature, double based rocket propellants may undergo the degradation of their mechanical properties, which can significantly influence their stability. Because of safety reasons, it is necessary to establish an appropriate method for the prediction of the propellants behaviour over a long-term period of time under defined temperature conditions. Applying accelerated temperature measurements and time-temperature superposition (TTS) treatment of the data, limited lab testing (creep or stress relaxation) is sufficient to project long-term properties under different conditions. Dynamic mechanical analysis, which measures the modulus and damping properties of material, is one of the most convenient thermal analysis techniques that can be applied for time-temperature superposition approach. The goal of this work was to investigate the applicability of the TTS principle to the prediction of the mechanical properties of double based rocket propellants during the ageing. The master curve was generated on the basis of the creep measurements in the temperature region from -71 to +20°C, by a dynamic mechanical analyser. The generated master curve was mathematically described by Williams-Lander-Ferry (WLF) and Arrhenious models. Material constants in the WLF equation were determined to be C1=44.43 and C2=308.4, and the viscoelastic activation energy from the Arrhenious equation was determined to be Ea= 152.7 kJ/mol. The results have shown that the TTS principle is applicable to the prediction of the propellants behaviour during a long-term period of time at defined temperature conditions.
NTREM, PARDUBICE, 2005 page 663-673

INFLUENCE OF OIL ON SENSITIVITY AND THERMAL STABILITY OF TRIACETONE TRIPEROXIDE AND HEXAMETHYLENETRIPEROXIDE DIAMINE

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Abstract:
The desensitization of triacetone triperoxide (TATP) and hexamethylenetriperoxide diamine (HMTD) was investigated. WD-40 oil was used as a possible candidate. The sensitivity to friction and impact were studied for pure TATP and HMTD as well as mixtures with varying ratio of WD-40 oil. Thermal stability of such mixtures was determined using DTA.
NTREM, PARDUBICE, 2005 page 674-679

EFFECT OF ALUMINIUM POWDER ON THE THERMAL AND ENERGETIC PROPERTIES OF COMPOSITE ROCKET PROPELLANT BASED EPOXY RESIN

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Abstract:
The objective of this work is to study the effect of aluminium rate on the thermal, kinetic and energetic properties of catalysed composite propellant based DGEBA epoxy resin binder. The first part of this study is consisting of the formulation of the propellant at different rates of the aluminium powder (from 0 to 20 % in weight), and by incorporation copper chromite as burning catalyst. The second part consists to characterize thermally, kinetically and energetically the propellant samples by using DSC (auto-inflammation temperature), TGA (activation energy) and adiabatic calorimeter (calorific potential) of the elaborated propellant.
NTREM, PARDUBICE, 2005 page 680-686

CRYSTALLIZATION OF HEXANITROSTILBENE

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Abstract:
In this paper, the method of synthesis and crystallizations of hexanitrostilbene are presented. The aim of the work was to obtain cubic crystals of HNS. Several solvents for crystallization of HNS were checked. The 100% fuming nitric acid as a solvent to crystallization was the best. The influence of various parameters on crystallization process was investigated. The particle size distribution and the tap density in the crystals obtained are presented.
NTREM, PARDUBICE, 2005 page 687-694

CHARACTERIZATION OF COMPOSITE SOLID ROCKET PROPELLANT USING DMA

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Abstract:
Dynamic mechanical analysis has been used to characterize mechanical properties of selected composite solid rocket propellant. Different experimental approaches to obtain data for determination of activation energies Ea associated with glass transition are presented. The experimental results show that the Ea values differ depending on the method used for evaluation. Some limitations of the time temperature superposition principle are discussed.
NTREM, PARDUBICE, 2005 page 695-707

AN ANALYSIS OF BLAST WAVES PARAMETERS AND UNDERWATER EXPLOSION TEST OF EMULSION EXPLOSIVES AND DYNAMITES

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Abstract:

In the paper results of experimental investigations as well as numerical analyses of blast waves parameters and underwater explosion test results of water-in-oil emulsion explosives and dynamites is presented. In the experiments the overpressure magnitude in transient shock wave generated by explosion of investigated explosives in air and in water as well as time of bubble collapse was measured. Also numerical evaluation of blast field in the space surrounding the explosive charge is performed. Comparison of the blast wave intensity generated by various kinds of explosives with underwater explosion test results is performed.

NTREM, PARDUBICE, 2005 page 708-718

SOPHISTICATED ELECTROCATALYSTS FOR ECONOMICAL PRODUCTION OF HYDROGEN PART A: STRUCTURAL CHARACTERIZATION

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Abstract:

An original procedure was applied in order to prepare composite electrocatalysts for hydrogen evolution reaction (HER), containing Ni, Co and CoNi as a hyper delectronic phase and TiO_2 as a hypo-phase deposited on conductive carbon substrate Vulcan XC-72. The catalyst’s support (TiO2 and carbon) was thermally treated on 250 and 480oC in the atmosphere of H2 and N2. XRD and SEM methods were employed in order to elucidate the influence of temperature on the structural characteristics of catalysts.

XRD analysis has shown that all catalysts contain hyper d-metallic phase of crystalline structure, the size of grains being 10¸20 nm, except the Co-phase that showed to be amorphous (grain size < 2 nm). TiO2 calcinated on 480°C has shown typical anatase structure, while no crystalline state was observed for that calcinated on 250°C.

For all types of catalysts, an aggregation of grains in clusters of a size of typically 100 nm was observed by SEM analysis. Also, a presence of empty space, that improves material’s porosity and specific surface area respectively, has been shown. Further improvements of the non-platinum hypo-hyper d-catalysts are in course.

NTREM, PARDUBICE, 2005 page 719-729

ESTIMATION OF THE CONDENSATION PROBABILITY OF SUPERSATURATED NITROGLYCERINE VAPOR DURING MANUFACTURING OF ENERGETIC MATERIALS

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Abstract:
Thermodynamic conditions for the condensation of supersaturated nitroglycerine vapor on the cold surfaces of apparatus during energetic materials manufacturing are analyzed. The tendencies in condensation center generation upon cooling of onecomponent (nitroglycerine) and two-component (nitroglycerine + coplasticizer) vapor are considered. The use of a two-component plasticizer reduces the probability of liquid plasticizer drops appearing on the apparatus surface.
NTREM, PARDUBICE, 2005 page 730-738

SOPHISTICATED ELECTROCATALYSTS FOR ECONOMICAL PRODUCTION OF HYDROGEN PART B: ELECTROCHEMICAL CHARACTERIZATION

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* Faculty of Technology and Metallurgy, University "Sts. Cyril and Methodius", Skopje, R. Macedonia
** Military Academy "Mihailo Apostolski", Skopje, R. Macedonia

Abstract:
Electrochemical characterization of composite hypo-hyper d- electrocatalysts for hydrogen evolution reaction (HER) was performed using cyclic voltammetry and steadystate galvanostatic method. Cyclic voltammograms are without any pronounced peaks corresponding to some surface processes, typically for porous electrodes. The influence of the temperature on electrocatalytic activity was studied. The catalysts with support treated on 480°C are more active than those on 250°C. The overpotential difference ($\eta_{250°C} - \eta_{480°C}$) for hydrogen evolution at 60 mA·cm^{-2} is 15 mV for Co based electrocatalyst and even 60 mV for Ni based. Comparing the electrocatalytic activity of the catalysts with different hyper d-metallic phase, one can conclude that the activity decreases in the sequence: Co > CoNi > Ni. Evidence is produced that the investigated non-precious catalysts show significant synergetic effect. These results are valuable per se and also as indicators for further improvement of non-platinum hypo-hyper d-catalysts.
NTREM, PARDUBICE, 2005 page 739-744

COMPARISON OF MEASURED AND CALCULATED PARAMETERS OF PROPELLANTS

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Abstract:
This paper deals with comparison of experimentally observed and calculated values of heat of explosion of several propellant compositions. For calculations „TCHAR©" program was used.
NTREM, PARDUBICE, 2005 page 745-749

CHANGES OF SOME THERMOPHYSICAL PROPERTIES OF NITROCELLULOSE PROPELLANTS DURING ACCELERATED AGING

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Abstract:
The ageing of nitrocellulose propellants causes changes of a number of relevant propellants properties (decrease of nitrocellulose molar mass, decrease of stabiliser content, change of thermophysical properties, etc.). The quality of propellants at a given moment of time, i.e. their stability, may be determined by measuring these properties. The changes of some thermophysical properties of nitrocellulose propellant during accelerated aging have been studied in this paper applying differential scanning calorimetry (DSC). The series of nitrocellulose propellant sample were aged in temperature range between 80 up to 100 °C. It was found out that some DSC parameters of aged nitrocellulose propellants differ significantly (temperature of maximum and width at half height of DSC peak increase, height and reaction enthalpy decrease). This suggests that the information derived from DSC measurements can help in nitrocellulose propellant stability evaluation.
NTREM, PARDUBICE, 2005 page 750-756

ON THE ESTIMATION OF COOKOFF TEMPERATURE USING FEM

Jakub Šelešovský, and Jiří Pachmáň
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Abstract:
The simulation of temperature distribution during cookoff is presented in this paper. Cylinder charge of RDX in steel confinement was heated by heating rate 3 K.hr-1. The ignition was predicted at the temperature 160°C and occurred in the central part of the charge. The simulation was carried out using the ANSYS Multiphysics finite element code.
NTREM, PARDUBICE, 2005 page 757-763

HAZARD OF EXOTHERMAL REACTIONS IN PRODUCTION OF NITROCOMPOUNDS

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Abstract:
Hazard of runaway of nitration processes in nitrocompounds production was investigated. Temperature rise in DNT nitration mixes under near adiabatic conditions was measured, and derivative dT/dt was computed. Heat evolution rate caused by nitration (primary reaction) and oxidation (secondary reaction) were examined by mathematical model. Limiting values of T and dT/dt for safe process were determined.
NTREM, PARDUBICE, 2005 page 764-770

THEORETICAL STUDIES ON THE PROPERTIES OF SOME ENERGETIC MATERIALS

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Abstract:
The theoretical results of structure-sensitivity relationship of several energetic materials were introduced. It is demonstrated that the nitro group charges can be used to assess impact sensitivity like bond length, oxygen balance and molecular electrostatic potential. When nitro group Mulliken charges less than 0.23e, the compound may have H50.0.4m. In addition, the thermal properties and the detonation performance of single and multi furazans and furoxans compounds were introduced. The results suggested that those compounds have high energy and relatively high sensitivity. They are the important compounds in the viewpoint of high energy density materials designing.

NTREM, PARDUBICE, 2005 page 771-780

INFLUENCE OF VELOCITY OF GAS FLUX GOING TO EROSIVE BURNING PROCESS INSIDE OF COMBUSTION CHAMBER

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Abstract:
This paper includes the results 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 University of Defense in Brno and members of Explosia, a.s. provided the realization of these tests.

NTREM, PARDUBICE, 2005 page 781-788

DETERMINATION OF NITRATE ESTERS CONTENT IN WATER SAMPLES

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Abstract:
This paper describes a method for the analysis a mixture of nitroglycerin (NG) and ethylene glycol dinitrate (EGDN) in water samples. Nitroglycerin has used in explosives – in many dynamites and multi-base propellants. Nitrate esters low contents were determined with two extraction techniques – solid phase extraction (SPE) and solid phase microextraction (SPME). Several types and adsorbents of the SPE columns were tested. SPME parameters including adsorption and desorption time, coating type, rate of stirring and salt addition were optimized. After extraction the analytes were separated and quantified using high-pressure liquid chromatography with ultraviolet detection (HPLC/UV).

NTREM, PARDUBICE, 2005 page 789-794

IDENTIFICATION AND MUTUAL DIFFERENTIATION BETWEEN NITROESTERS AND NITRAMINES BY THE COLOUR REACTION WITH THYMOL

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Abstract:
In the present paper there is discussed the colour reaction of nitramines and nitroesters with thymol what can be used for their mutual differentiation. The reaction is supplemental to these employed in commercial kits for detection of explosives. It was examined in different modifications – as a spot test, a test-tube reaction and also on filters.
NTREM, PARDUBICE, 2005 page 795-801

UV-VIS SPECTRA OF SOME ENERGETIC MATERIALS MEASURED WITH THE OPTICAL FIBER PROBE

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Abstract:
The present paper is focused on possibilities of identification of explosives or their decomposition products using the UV-Vis spectrometry. The spectral analysis is employed there in the region of 200-800 nm. The spectra were measured using the optical fibre probe what is especially set for powders and thick fluids.
NTREM, PARDUBICE, 2005 page 802-807

DIFFERENTIAL SCANNING CALORIMETERS

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Abstract:
In this paper the principles are outlined of differential scanning calorimetry. Main characteristics that can be determined by means of this method are listed. Examples of results are presented of thermal stabilities of some explosives.
NTREM, PARDUBICE, 2005 page 808-815

STRUCTURE-KINETIC LAWS OF THERMAL DECOMPOSITION OF SIX-MEMBERED CYCLIC N-NITRAMINES

Rudolf S. Stepanov, Ludmila A. Kruglyakova, and Alexander M. Astachov
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Abstract:
The thermal decomposition of six-membered cyclic N-nitramines, contained in ring one, two and three nitramine fragments, and also oxy-, gem-dinitro, azido and tetrazole function, is investigated, using manometer method combined with chromatography, FTIR-spectroscopy and mass-spectrometry. Influence of functional groups on the rate and activation parameters of N-nitramine's decomposition limited stage is established.
NTREM, PARDUBICE, 2005 page 816-824

RECORDING OF PARTICLE VELOCITY PROFILES IN SHOCK AND DETONATION WAVES BY ELECTROMAGNETIC TECHNIQUE

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Abstract:
The electrocontact and photochronographic procedures were used to study detonation propagation in cylindrical samples of different diameter made of insensitive HE for the cases of single-point and plane-wave initiation. The diameter of samples ranged from 15 to 120mm. The stationary detonation rate vs diameter of the cylindrical sample was constructed. The relation between the curvature of the detonation front and its rate is identified
NTREM, PARDUBICE, 2005 page 825-831

THE USE OF THE GAP TEST TO INVESTIGATE THE SHOCK TO DETONATION TRANSITION IN LOW-SENSITIVITY EXPLOSIVES PART I – EXPERIMENTAL APPROACH

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Abstract:
In the present work an attempt was undertaken to apply the gap test configuration for investigation of the process of buildup of detonation in low-sensitivity explosives. The set-up was proposed in which sensitivity on shock wave and shock wave velocity can be measured simultaneously. The detonation initiation was investigated in the compositions containing 3-nitro-1,2,4-triazol-5-on (NTO).
NTREM, PARDUBICE, 2005 page 832-838

THE USE OF THE GAP TEST TO INVESTIGATE THE SHOCK TO DETONATION TRANSITION IN LOW-SENSITIVITY EXPLOSIVES PART II – NUMERICAL SIMULATION

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Abstract:
In the present work the process of shock to detonation transition in the gap test configuration was modelled. The reacting explosive was approximated by a twocomponent gas-solid medium. To describe the rate of chemical transformation of the explosive, the three-term macrokinetic equation was applied. The results of modelling were compared with the gap test data.
NTREM, PARDUBICE, 2005 page 839-845

AGING BEHAVIOR OF PROPELLANTS

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Abstract:
Nitrocellulose is used as a main component of propellants. The aging behavior of various type of nitrocellulose were studied at the neighborhood of room temperature from 25 degrees to 50 degrees by accelerating aging tests. Moreover, the aging behavior of propellants which contained stabilizers was also investigated using four kinds of stabilizers such as ethylcentralite, diphenylamine, 2-nitrodiphenylamine and akardite 2 in this study. From these results, the reason of degradation of nitrocelulose and propellant were ascribed to acid hydrolysis and peroxide formation.
NTREM, PARDUBICE, 2005 page 846-852

CONTRIBUTION TO STUDIES OF DETONATION OF A CURVED CYLINDRICAL CHARGE

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Summary*:*
In connection with previous experiments and newly gained knowledge there have been suggested and realized experiments, which should have better involved the character of process of the detonation wave influenced by the way of deformation of cylindrical charge made from a special plastic explosive on RDX basis. The character of process of the detonation wave has been researched in connection with done experiments by the help of the numerical simulation method – Finite Element Method in Lagrangian system ANSYS/LS-DYNA 3D.
NTREM, PARDUBICE, 2005 page 853-863

APPLICATION OF LC-MSD AND GC-ECD TECHNIQUES IN THE ANALYSIS OF POST EXPLOSION RESIDUES OF EXPLOSIVES ON THE BASIS OF 1,3,5-TRINITROSO-1,3,5-TRIAZINANE

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Abstract:
The paper deals with possible applications of the connection of liquid chromatography with atmospheric pressure chemical ionization (APCI) mass spectrometry (Agilent 1100 series LS-MSD system) and gas chromatography with electron capture detector (GC-ECD) in the analysis of some common available or improvised explosives. The analysis of slected types of individual explosives, 2,4,6-trinitrotoluene (TNT), 1,3,5-trinitroso-1,3,5-triazinane (TMTA) and analysis of their mixtures (TNT/TMTA and RDX/TMTA) in their post explosion residues on the basis of generated characteristic mass spectra by using LC-MSD system is the aim of this work.
Post explosion analysis of TMTA and its explosive mixtures can be similarly complicated, like that of the well-known plastic explosive on the basis of pentaerythritol tetranitrate, Semtex-1A.
NTREM, PARDUBICE, 2005 page 864-874

INTERMOLECULAR INTERACTIONS OF ENERGETIC COMPOUNDS IN GASEOUS AND SOLID STATES

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Abstract:
The first-principle methods were applied to the study of some energetic compounds in both gaseous dimer and bulk state. The binding energies have been corrected for the basis set superposition errors. The influences of molecular interactions on the molecular properties were discussed. The lattice energies, electronic band structures and density of states in the solid states were obtained. Relationship between the electronic structures and some detonation characteristics were elucidated.
NTREM, PARDUBICE, 2005 page 875-888

SYNTHESIS AND APPLICATION OF GEMINI SURFACTANT IN EMULSION EXPLOSIVE

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Abstract:
Cationic Gemini Surfactant was synthesized from N,N-dimethyldodecyltertamine and 1,3-dibromopropane by using ethanol as solvent. After being recrystallized from the ethyl acetate-ethanol solvent mixture, the Gemini product was qualitatively detected and verified by IR and 1HNMR. The emulsion explosive, which uses the Gemini surfactant as crystal modifier and auxiliary emulsifier, has smaller W/O type particle size and better distribution, stability and explosion properties.
NTREM, PARDUBICE, 2005 page 889-895

EFFECTS OF THE REACTION OF THE LINER CONTAINING THE MAGNESIUM AND ALUMINUM WITH WATER AND WATER SOLUTION OF AMMONIUM NITRATE

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The article presents part of research on axial -direction shaped charges - with metal powder liners containing powders of aluminum and magnesium. We are presenting the idea of the association of the cumulative effect with the additional energetic effect. These effects are possible to obtain by using proper chemical constitution liners. We present effects obtained on the blasting ground.
NTREM, PARDUBICE, 2005 page 896-900

STUDY OF THERMAL AND DETONATION REACTIVITIES OF THE MIXTURES CONTAINING 1,3,5-TRINITROSO-1,3,5-TRIAZINANE (TMTA)

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Abstract:
Thermal reactivities of 1,3,5-trinitroso-1,3,5-triazinane (TMTA), 1,3,5-trinitro-1,3,5-triazinane (RDX), 2,4,6-trinitrotoluene (TNT), TNT/TMTA and RDX/TMTA mixtures and mixtures of 1,3,5-trinitrobenzene (TNB) with TMTA and TMTA/RDX were specified by means of differential thermal analysis with outputs evaluation by the Kissinger method. The reactivities, expressed as Ea R-1 slopes of Kissinger relationship, correlate with squares of detonation velocities of the corresponding explosive samples in the sense of modified Evans-Polanyi-Semenov equation. Taking this fact it is stated that initiation of detonation of the mixtures with TMTA content proceeds through primarily fission of the TMTA molecule. If an ionic mechanism dominantly participates on thermal decomposition of some studied mixtures then resulting Ea R-1values do not correlate in the sense of the equation. This is the case of the TNT/TMTA mixtures where TNT has acidic character toward TMTA. Also in TNB/TMTA/RDX mixture might react amine intermediates of TMTA thermal decomposition with RDX by ionic mechanism.
NTREM, PARDUBICE, 2005 page 901-909

STUDY ON MECHANISMS OF INITIATION OF TWO POLYNITRO ARENES

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Abstract:
Each from the 2,6-bis(2,4,6-trinitrophenylamino)-3,5-dinitropyridine (PYX) and 2,4,6-tris(3-methyl-2,4,6-trinitrophenylamino)-1,3,5-triazine (TMPM) molecules contains two potential centres of the primary fission in its initiation. This fission should be realized by the migration of .-hydrogen atom to oxygen atom of ortho-nitro group ("trinitrotoluene mechanism"). Taking of the relationships between impact sensitivity and 13C NMR chemical shits of some polynitro arenes and between Mulliken charges on nitrogen atoms of primarily reacting nitro group and onsets from differential thermal analysis of the said compounds, with the aid of DFT-B3LYP/3-21G methods of GAUSSIAN 98/03 program, the more probable pathways of initiation of the above-mentioned molecules are estimated.
NTREM, PARDUBICE, 2005 page 910-916

COMPARISON OF CONTINOUS AND DISCONTINOUS METHOD OF DETONATION VELOCITY MEASUREMENT IN MINING DRILLS (VOD)

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Abstract:
Detemination of caracteristics of explosives – detonation velocities in mining drills by continuous and discontinous method performed in "Črnotići" quary. Measurements are performed in same mine field – therefore under geologically exactly same conditions. Data retrieved show difference between mentioned measurement methods and works and measurement principles themselves. Detonation velocitiy measurement following discontinuous method was performed on semi-highway track "Bar – Podgorica" on section "Tanki rt – Đurmani". Measurements were conducted in different length of measurement intervals for mining drill charges, with results confirming conclusions obtained by continuous method measurements.
NTREM, PARDUBICE, 2005 page 917-924

NON STANDARD METHODES IN TESTING FIRING CURRENT OF ELECTRIC DETONATORS

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Abstract:
For testing electrical detonators some countries have national standards, members of the European Union have drafts or accepted standards that describe equipment minimal electrical and mechanical properties, preparation of samples to be tested, handling and testing procedures and finally data processing and presentation. In this paper we will consider one alternative method for testing firing current of electrical detonators and compare it to standard method of testing.
NTREM, PARDUBICE, 2005 page 925-931

COMPARISON OF VOD MEASUREMENT RESULTS WITH CONTINUOUS AND DISCONTINUOUS METHOD

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Abstract:
An explosive´s velocity of detonation (VOD), can be used to indicate a number of important characteristics regarding the product´s performance under specific field and test conditions. A number of charasteristic and transient VOD curves have been identified, which can be used to evaluate explosive performance, control ground vibration amplitudes, select the correct amount and type of stemming, eliminate explosive desensitization and evaluate primer performance. Although the primary focus of this paper is comparison of VOD measurement results with continuous and discontinuous method.
NTREM, PARDUBICE, 2005 page 932