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| 12. PERSONAL AUTHOR(S) C. B. Storm, and T. B. Brill | | | | | | |
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| FIELD | GROUP | SUB-GROUP | | | | |
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| 19. ABSTRACT (Continue on reverse if necessary and identify by block number) A Gordon Research Conference on the Chemistry of Energetic Materials was held at the New Hampton School 27 June - 1 July 1988. There were 110 attendees. A broad range of topics were covered: reactions in energetic materials, modeling in reactive systems, equation of state, structural chemistry, thermal decomposition, new materials, spectroscopy in fast reactions, and chemistry at high pressure. There were 28 speakers who were recognized leaders in their technology areas. There were 40 poster papers on diverse topics. | | | | | | |
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| 22a. NAME OF RESPONSIBLE INDIVIDUAL Dr Anthony J. Matuszko | | | 22b. TELEPHONE (Include Area Code) (202) 767-4963 | | 22c. OFFICE SYMBOL AFOSR/NC | |

**1988 GORDON RESEARCH CONFERENCE ON THE
CHEMISTRY OF ENERGETIC MATERIALS**

FINAL PROGRESS REPORT

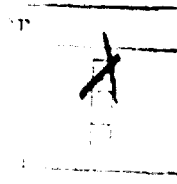
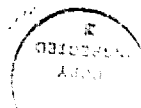
GRANT AFOSR-88-0193

The Gordon research Conference on "The Chemistry of Energetic Materials" was held from June 27 to July 1, 1988 at the New Hampton School, New Hampton, New Hampshire. The conference had 110 participants, 13 per cent from foreign countries. There was a good mixture of scientists from universities, national laboratories, DoD laboratories, research institutes and private industry, including young scientists, graduate students, and postdoctoral associates as well as established scientists.

The program for the conference brought together research scientists working in several different areas, who share a common interest in the basic chemistry and physics of the performance and safety of energetic materials. The topics discussed included: Reactions in Energetic Materials, Modeling in Reactive Systems, Equation of State, Structural Chemistry, Thermal Decomposition, New Materials, Spectroscopy in Fast Reactions and Chemistry at High Pressure. The discussion following the talks was extensive and continued beyond the sessions into the afternoon and evening into the free time scheduled for the conferees. There was a poster session at which forty posters were presented. The posters were put up Tuesday afternoon and active discussion the the contents continued for the week.

Much of the discussion at the conference centered around the idea of what is the chemical speciation that takes place in the predetonation period, during the detonation and in a propellant burn. Central questions were addressed as to how these species can be detected spectroscopically, how they can be predicted from theoretical calculations, how they can be used in modeling the reaction and constructing kinetic models for the behavior of various energetic materials. Consideration was given to the role of molecular and crystal structure in predicting performance and understanding reactivity.

The general comments of the conferees was that it was a very successful Gordon Research Conference and a second conference has been requested for the summer of 1990. The 1990 conference will be Chaired by Professor Thomas B. Brill, Department of Chemistry, University of Delaware. Dr. Christos Capellos, US ARDEC, Dover, NJ was elected Vice Chairman of the 1990 conference.



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GORDON RESEARCH CONFERENCE
CHEMISTRY OF ENERGETIC MATERIALS
NEW HAMPTON SCHOOL, NEW HAMPSHIRE
JUNE 27 - JULY 1, 1988

C. B. Storm, Chairman

T. B. Brill, Vice Chairman

PROGRAM SCHEDULE

Monday, June 27

7:45 AM BREAKFAST

8:30-8:40 AM, Welcome and organizational comments, C. B. Storm.

SESSION 1. REACTIONS IN ENERGETIC MATERIALS, J. P. RITCHIE, DIS. LDR.

8:40-9:15 AM, J. P. RITCHIE, THEORETICAL CALCULATIONS OF THE STRUCTURE, ENERGY AND REACTIONS OF EXPLOSIVES.

9:15-9:25 DISCUSSION

9:25-10:00 J. R. MURDOCH, REACTIVITY AND THERMODYNAMICS OF ENERGETIC MATERIALS. PREDICTIONS FROM EXPERIMENTAL DATA.

10:00-10:10 DISCUSSION

10:10-10:30 COFFEE BREAK AND GROUP PHOTOGRAPH

10:30-11:05 C. F. MELIUS, REACTION MECHANISMS IN THE IGNITION AND COMBUSTION OF NITRAMINES.

11:05-11:15 DISCUSSION

11:15-11:50 P. GRAY, THERMAL FEEDBACK AND INSTABILITIES.

11:50-12:10 DISCUSSION

12:30 LUNCH

6:00 PM DINNER

SESSION 2. MODELING IN REACTIVE SYSTEMS, D. S. STEWART, DIS. LDR.

7:30-8:05 PM, J. B. BDZIL, STATE-DEPENDENT REACTION RATES: THEIR ROLE IN DETERMINING THE STRUCTURE OF THE DETONATION REACTION ZONE.

8:05-8:15 DISCUSSION

8:15-8:45 D. S. STEWART, DETONATION STABILITY.

8:45-8:55 DISCUSSION

8:55-9:10 BREAK

9:10-9:45 D. KASSOY, A COMPARISON BETWEEN DIFFUSIVE AND NONDIFFUSIVE THERMAL EXPLOSION PHENOMENA.

9:45-9:55 DISCUSSION

TUESDAY, JUNE 28

7:45 AM BREAKFAST

SESSION 3. EQUATION OF STATE, J. D. JOHNSON, DISC. LDR.

8:30-9:10 AM F. H. REE, MULTIPHASE MIXTURE EOS UNDER REACTIVE AND NONREACTIVE ENVIRONMENTS.
9:10-9:20 DISCUSSION
9:20-10:00 W. BYERS BROWN, THE EFFECTS OF CHEMISTRY AND PHASE CHANGES ON THE IDEAL DETONATION STATE.
10:00-10:10 DISCUSSION.
10:10-10:30 COFFEE BREAK
10:30-11:10 M. S. SHAW, DENSE FLUID EQUATION OF STATE: THEORY AND SIMULATIONS.
11:10-11:20 DISCUSSION
11:20-12:00 J. D. JOHNSON, CARBON COAGULATIONS IN DETONATIONS.
12:00-12:10 Discussion
12:30 LUNCH

4:30-6:00 PM POSTER SESSION

6:00 DINNER

SESSION 4. STRUCTURAL CHEMISTRY, H. AMMON, DISC. LDR.

7:30-8:15 PM J. HOLDEN, PREDICTION OF CRYSTAL STRUCTURE FROM MOLECULAR CONFORMATION.
8:15-8:25 DISCUSSION.
8:25-8:40 BREAK
8:40-9:25 C. LOWE-MA, DOES THE CRYSTAL STRUCTURE PLAY A ROLE IN AN ENERGETIC MATERIALS PROPERTIES?
9:25-9:35 DISCUSSION

WEDNESDAY, JUNE 29
7:45 AM BREAKFAST

SESSION 5, THERMAL DECOMPOSITION, T. B. BRILL, DISC. LDR.

8:30-9:10 AM T. B. BRILL, FAST THERMAL DECOMPOSITION CHEMISTRY.
9:10-9:20 DISCUSSION
9:20-10:00 A. C. ECKBRETH, NEW CONCEPTS FOR CARS DIAGNOSTICS OF SOLID PROPELLANT COMBUSTION.
10:10-10:10 DISCUSSION
10:10-10:30 COFFEE BREAK
10:30-11:10 X. ZHAO, CONCERTED DISSOCIATION IN RING COMPOUNDS.
11:10-11:20 DISCUSSION
11:20-12:00 R. BEHRENS, INVESTIGATIONS OF HMX AND RDX THERMAL DECOMPOSITIONS WITH SIMULTANEOUS THERMOGRAVIMETRIC MODULATED MOLECULAR BEAM MASS SPECTROMETRY ANALYSIS.
12:00-12:10 DISCUSSION
12:30 LUNCH

4:30-6:00 PM BUSINESS MEETING.

6:00 DINNER

SESSION 6, NEW MATERIALS, D. McMillen, DISC. LDR.

7:30-8:05 PM A. T. NIELSEN, SYNTHESIS OF CAGED NITRAMINE COMPOUNDS
8:05-8:15 DISCUSSION.
8:15-8:50 P. E. EATON, NEW WORK WITH THE CUBANE SYSTEM.
8:50-9:00 DISCUSSION
9:00-9:15 BREAK
9:15-9:50 R. SCHMITT, HYPOTHETICAL STRUCTURES FOR EXPLOSIVES AND PROPELLANTS.
9:50-10:00 DISCUSSION

THURSDAY, JUNE 30

7:45 AM BREAKFAST

SESSION 7, SPECTROSCOPY IN FAST REACTIONS, A. M. RENLUND, DISC. LDR.

8:30-9:10 AM C. WITTIG, PHOTOINITIATED REACTIONS IN UNIQUE ENVIRONMENTS.
9:10-9:20 DISCUSSION
9:20-10:00 W. TROTT, REAL-TIME SPECTROSCOPIC STUDIES OF SHOCKED ENERGETIC MATERIALS.
10:00-10:10 DISCUSSION
10:10-10:30 COFFEE BREAK
10:30-11:10 S. DUFORT, THE USE OF TIME RESOLVED SPECTROSCOPIES IN THE STUDY OF THE INITIATION OF EXPLOSIVES AT THE MOLECULAR LEVEL.
11:10-11:20 DISCUSSION
11:20-12:00 K. EISENTHAL, LASER STUDIES OF ULTRA-FAST PROCESSES IN LIQUIDS.
12:00-12:10 DISCUSSION
12:30 LUNCH
6:00 PM DINNER

SESSION 8, 7:30 PM, W. C. DAVIS, OUTSTANDING PROBLEMS IN DETONATION SCIENCE; FOLLOWED BY A PANEL DISCUSSION: G. A. LEIPER, R. S. MILLER, A. M. RENLUND.

FRIDAY, JULY 1

7:45 AM BREAKFAST

SESSION 9, CHEMISTRY AT HIGH PRESSURE, S. TREVINO, DISC. LDR.

8:30-9:10 AM P. MILLER, EFFECTS OF PRESSURE AND TEMPERATURE ON THE
KINETICS AND CHEMICAL REACTIVITY OF NITRAMINE
EXPLOSIVES.
9:10-9:20 DISCUSSION
9:20-10:00 M. NICOL, REACTIONS AND STRUCTURES OF SOME
UNSATURATED H-C-N-O SOLIDS AT HIGH STATIC AND
DYNAMIC PRESSURES.
10:00-10:10 DISCUSSION
10:10-10:30 COFFEE BREAK
10:30-11:10 S. AGNEW, HIGH PRESSURE REACTIONS OF ENERGETIC
MATERIALS: NITROMETHANE AND NITRIC OXIDE.
11:10-11:20 DISCUSSION

LUNCH & DEPARTURE.

GORDON RESEARCH CONFERENCE
CHEMISTRY OF ENERGETIC MATERIALS
NEW HAMPTON SCHOOL, NEW HAMPSHIRE
JUNE 27 - JULY 1, 1988

POSTER SESSION
TUESDAY, JUNE 28, 1988; 4:30-6:00 PM

H. L. AMMON AND R. W. ARMSTRONG, MODELING STUDIES OF RDX AND HMX CRYSTAL DEFORMATIONS.

R. C. ARMSTRONG, CHEMICAL AND HYDRODYNAMIC CONTRIBUTIONS TO LIQUID MONOPROPELLANT STABILITY.

A. BASHIR-HASHEMI, NEW DEVELOPMENTS IN CUBANE CHEMISTRY - PHENYL CUBANES.

B. C. BEARD AND J. SHARMA, RADIATION SENSITIVITY AND DECOMPOSITION OF NTC

N. BLAIS, THE FREE EXPANSION OF DETONATION PRODUCTS IN VACUUM.

P. BRUSH AND T. B. BRILL, FAST HEAT AND HOLD DECOMPOSITION OF HMX AND RD

F. BUGAUT, THERMODYNAMICS OF DENSE FLUID NITROGEN BY MONTE CARLO SIMULATION.

R. J. BUTCHER, A. OKONKOW, N. S. ROWAN-FORDON AND A. NGUYEN-PHO, EACAILE ELECTROPHILIC SUBSTITUTION IN METAL ION COORDINATED HETEROCYCLES.

R. S. DAMAVARAPPU AND S. IYER, SYNTHETIC DESIGNS TOWARDS POLYNITROPOLYHEDRANES.

L. R. DOSSER, LASER ILLUMINATED HIGH SPEED PHOTOGRAPHY OF ENERGETIC MATERIALS.

L. R. DOSSER, LASER IGNITION OF ENERGETIC MATERIALS.

C. H. DOUGLAS AND J. K. RICE, NASCENT BH DISTRIBUTIONS FROM THE PHOTODISSOCIATION OF BH₃CO AT 193 nm.

W. ELBAN, P. J. COYNE, JR., R. W. ARMSTRONG, H. W. SANDUSKY, B. C. GLANCY, AND D. W. CARLSON, BIG POINTS FROM SMALL IMPRESSIONS IN AMMONIUM PERCHLORATE.

D. W. FIRSICH, POLYMORPHISM IN HEXANITROAZOBENZENE.

M. F. Foltz and C. B. Moore, PHOTOFRAGMENT DYNAMICS OF FORMALDEHYDE.

M. J. B. GREEN, M. J. PILLING AND S. H. ROBERTSON, DIFFUSION AND DETONATION.

J. A. HOLY AND T. C. GIRMANN, THE EFFECTS OF PRESSURE ON THE LASER INITIATION OF $TiH_x/KClO_4$ AND OTHER PYROTECHNICS.

S. R. JAIN, PREIGNITION REACTIONS IN HYPERGOLIC SYSTEMS.

K. JAYASURIYA AND O. SANDUS, EFFECT OF SUBSTITUENT GROUPS ON STRAIN ENERGY.

J. J. KAUFMAN, AB-INITIO MRD-CI CALCULATIONS FOR BREAKING A CHEMICAL BOND IN A MOLECULE IN A CRYSTAL OR OTHER SOLID ENVIRONMENT: NITROMETHANE.

S. Lambrakos, M. Peyrard and E. S. Oran, ANALYSIS OF MICROSCOPIC STRUCTURE OF DETONATIONS IN ENERGETIC SOLIDS.

J. F. LIEBMAN, J. S. CHICKOS, D. G. HESSE S. Y. PANSHIN AND K. A. GEORGIU, ESTIMATION OF HEATS OF VAPORIZATION AND SUBLIMATION OF ORGANIC COMPOUNDS.

W. L. LUKASAVAGE, A. BOHON, J. ALSTER AND S. NICOLICH, ISOTHERMAL PREPARATION OF 3,7-DIACETYL-1,3,5,7-TETRAAZABICYCLO-3.3.1-NONANE (DAPT).

A. P. MARCHAND, SYNTHESIS OF NOVEL POLYNITROPOLYCYCLIC COMPOUNDS: A NEW CLASS OF ENERGETIC MATERIALS.

R. W. MILLAR, NITRATION OF STRAINED RING COMPOUNDS.

R. MOWREY, THEORETICAL STUDY OF METHYLENENITRAMINE DECOMPOSITION.

S. ODIOT, DISSIPATION ENERGY AND DETONATION WAVE IN AN ENERGETIC MOLECULAR CRYSTAL.

V. R. PAI VERNEKER, ROLE OF CRYSTAL DEFECTS IN THE THERMAL REACTIVITY OF ENERGETIC MATERIALS.

P. PAPAGIANNAKOPOULOS AND C. CAPELLOS, KrF PHOTODECOMPOSITION OF TETRANITROMETHANE.

J. K. RICE, N. J. CALDWELL AND H. H. NELSON, REACTIONS OF BH.

R. C. Sausa, ELECTRONICALLY EXCITED SPECIES GENERATED BY EXCIMER LASER EXCITATION OF DIMETHYLNITRAMINE.

M. A. SCHROEDER, THERMAL DECOMPOSITION OF CATALYZED AND UNCATALYZED HMX PROPELLANT FORMULATIONS.

J. SHARMA, C. S. COFFEY, T. P. LIPPARD AND J. FORBES, CHEMICAL REACTIONS IN EXPLOSIVES PRECEDING IGNITION.

J. E. SHEPHERD, REACTION ZONE STRUCTURE IN GASEOUS MOLECULAR EXPLOSIVES.

G. P. SOLLOTT, POLYSUBSTITUTED ADAMANTANES EN ROUTE TO POLYNITROTRICYCLODECANES (ADAMANTANES), TRICYCLOOCTANES AND TRICYCLOHEXANES.

R. J. Spear, PARTICLE SIZE EFFECTS ON SHOCK SENSITIVITY OF RDX.

P. STEWART, J. B. JEFFRIES, J-M. ZELWEGGER, D. F. McMILLEN AND D. M. GOLDEN, LASER-POWERED HOMOGENEOUS PYROLYSIS OF DIMETHYLNITRAMINE DECOMPOSITION. GC/MS AND MOLECULAR BEAM/MS STUDIES.

C. B. STORM, ^1H - ^2H EXCHANGE IN NITROMETHANE.

J. H. STUFFLEBEAM, CARS APPLICATIONS TO SOLID PROPELLANT COMBUSTION.

H-t. WANG, C. Y. LIN AND M. C. LIN, THERMAL DECOMPOSITION OF NO_2 AND THE CHEMICAL KINETICS OF THE $\text{HCHO} + \text{NO}_2$ REACTION.

C-S. YOO, CHEMISTRY ON SHOCK COMPRESSED ORGANIC MOLECULES.

W. W. ZAJAC, TRANSFORMATION OF NITROGEN CONTAINING FUNCTIONAL GROUPS INTO NITRO GROUPS.

GORDON RESEARCH CONFERENCES
 ENERGETIC MATERIALS
 Carl Storm, Chairman
 New Hampton School
 June 27 - July 1, 1988

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| Carl F. Melius PO Box 969, Div 8357 Sandia National Lab. Livermore, CA 94550 415-294-2650 | BE 203 | | |

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