



1996 GORDON RESEARCH CONFERENCE

ON ENERGETIC MATERIALS

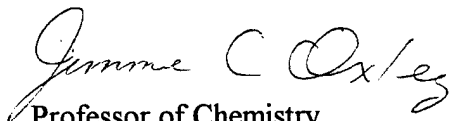
FINAL PROGRESS REPORT

GRANT NO: AFOSR F49620-96-1-0146

The Gordon Research Conference on Energetic Materials was held in New Hampton, NH at New Hampton School from 16 June to 21 June 1996. The Conference was well-attended with 117 in this field coming from academia, industry, and government laboratories, both U.S. and foreign scientists, senior researchers, young investigators, and students.

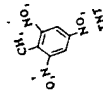
In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field. There was a conscious effort to stimulate lively discussion about the key issues in the field today. Time for formal presentations was limited in the interest of group discussions. In order that more scientists could communicate their most recent results, poster presentation time was scheduled. Attached is a copy of the formal schedule and speaker program and the poster program. In addition to these formal interactions, "free time" was scheduled to allow informal discussions. Such discussions are fostering new collaborations and joint efforts in the field.

I want to personally thank you for your support of this Conference. As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings. If you wish any further details, please feel free to contact me. Thank you.

  
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5th GORDON RESEARCH CONFERENCE  
**ENERGETIC MATERIALS**

June 16-21, 1996  
 New Hampton School, NH



Chair: Jimmie C. Oxley (URI)  
 Vice-Chairs: Steve Coffey (NSWC)  
 Anatoly Dremin (InstChemical Physics)

Financial support from:

- Gordon Research Conferences
- Sandia & Lawrence Livermore National Labs
- Office of Naval Research
- Air Force Office of Scientific Research
- Army Research Office
- TPL (reception)

**POSTERS 5th GRC on ENERGETIC MATERIALS**  
 IT Kraig Anderson (SNL, NM) "Thermal Decomposition of PETN"

- 2M James Barrett (NRL) "Effects of Crystalline Defects on the Initiation to Detonation Process in Model Energetic Materials"
- 3T Tod Botcher (City College, NY) & Tom Russell (NRL) "Pressure Dependence of the Decomposition of Condensed Phase RDX"
- 4T Haryuyuki Arisawa & Tom Brill (U Delaware) "Flash Pyrolysis Kinetics & Species of Azide Polymers: GAP"
- 5T Polly Gongwer & Tom Brill (U Delaware) "Flash Pyrolysis of Intimate Binder/Monopropellant Mixtures: RDX + CAB"
- 6T Ray Butcher; Rich Gilardi (NRL) "The Structure of Energetic Salts of Dinitramide with Main Group Transition Metal & Organic Cations"
- 7T Sury Bulusu (Piscataway, NJ); Rich Behrens (SNL, CA) "A Comparative Study of the Thermal Decomposition Mechanisms & Pathways of RDX, HMX, TNAZ, & Other Cyclic Nitramines"
- 8T Chris Capellos (Piscataway, NJ) "Ultrafast Decomposition in Energetic Nitramines" & "New Melt-Cast Formulations TNAZ"
- 9M C. Steve Coffey (NSWC) "Initiation by Impact or Mild Shock"
- 10M Arthur Cohen; R. A. Beyer "High Power Laser Ablation and Ignition of Solid Propellants"
- 11M Anatoly N. Dremin (Russia) "To the Intrafront Stage Reality at Detonation of Ideal Condensed Explosives"
- 12T Paritosh Dave (GeoCenters, NJ) "Acyliative Dealkylation of Azetidines: Application to Alternate Syntheses of TNAZ"
- 13M Richard Gilardi (NRL) "Crystal Structure & Density Nitro Cubanes"
- 14M W. Michael Howard & Laurence E. Fried (LLNL) "Kinetic Modeling of Non-Ideal Explosives with Cheestah"
- 15T Sampat R. Jain (India) "New Energetic Polymeric Binders"
- 16M Ed Kober (LANL) "Micromechanical Simulations of Plastic-Bonded High Explosives"
- 17T Sandor Kristyán & M.C. Lin (Emory, GA) "The Application of Energy Transfer & Tunneling to Reactions of Interest to Propellant Decomposition"
- 18M Joonbum Park & M.C. Lin (Emory, GA) "Mass-Spectrometric Studies of the NH<sub>2</sub>-NO<sub>x</sub> Chemistry for Mechanistic Elucidation of AN & AND Combustion Reactions"
- 19M Phil Pagoria (LLNL) "New Approaches to the Synthesis of

Inertive Energetic Materials"

- 20M Julian J. Lee & M. Brouillette (USherbrooke, QC, Canada) "Detonation Mechanisms in a Heterogeneous Condensed-Phase Explosive"
- 21T Leanna Minier; Richard Behrens (SNL, CA); Ted Burkey (U Memphis) "A Solid-Phase Thermal Decomposition Study of NTO Using Simultaneous Thermogravimetric Modulated Beam Mass Spectrometry (STMEMS)"
- 22M Indu Mishra (Howard U, Wash DC) & Tom Russel (NRL) Thermal Stabilization of AND"
- 23M Albert Nichols(LLNL) "Coupled Thermal Mechanical Chemical Modeling of Energetic Materials"
- 24T Weiyi Zheng; Jimmie Oxley; James Smith; Evan Rogers; Michael Coburn (U Rhode Island) "Thermal Decomposition Studies on TNAZ"
- 25T Xiaoxia Dong; Jimmie Oxley; James Smith; (U Rhode Island) "Kinetics and Mechanisms for Thermal Decomposition of NTO"
- 26M Tatyana S. Pivina; A.A. Porollo; E.V. Sokerina; V.A. Tartakovsky (Zelinsky Inst.; Russia) "Computer Modeling of Probable Decomposition Reactions for Energetic Compounds"
- 27M Alexandra Pilgrim (DRA, UK) "Novel Method for Chemiluminescence Detection of Explosives Traces"
- 28T Michael Schroeder (ARL) "Condensed-Phase Processes in Combustion of Solid Gun Propellants"
- 29M Ph. Simonetti (CEA, France) "Study of Explosive Initiation at a Molecular Level: Shock Wave & Electronic Structure"
- 30T D.C. Soressu; B.M. Rice; C. F. Chabalowski (ARL, MD); D. Thompson (Oklahoma,SU) "Intermolecular Potential for Cyclotrimethylene-trinitramine (RDX)"
- 31M Nirupam Trivedi (NSWC,MD) " Transannular Reactions in Syntheses of Difluoramine Based Energetic Materials"
- 32M Fred Volk (Fraunhofer Inst., Germany) "Detonation Products of Al-Containing High Explosives"
- 33T Shmuel Welner (ADA, Israel); Yehuda Hass; Y. Ben-Eliahu (Hebrew U, Jerusalem, Israel) "Initiation of GAP Decomposition by Pulsed IR & UV Laser"
- 34M D. Picart & R. Belmas (CEA FRANCE) "Pressed Explosives Mechanical Behavior, Damage, & Effects on Sensitivity--Experiments & Modeling"
- 35T K. L. McNesby (ARL) "Spectroscopic Determination of Impact Sensitivities of Explosives"

**Sunday Evening, June 16**

**Data Collection in Fast Reactions**

Discussant: Rich Behrens (Sandia, CA)  
7:30-7:50 Jane Rice (NRL) High-Pressure Matrix Isolation of Heterogeneous Reactions  
8:00-8:20 Tom Russell (NRL) Time-Resolved Optical Spectroscopy of Energetic Material Decomposition under Static High Pressure  
8:30-9:10 Vitaly Pepekina (Semenov Inst. Chem. Physics) & Boris Kondrikov (Mendeleev U ChemTech) Thermochemistry, Burning, & Detonation of Energetics Containing Nitrogen Acid Derivatives

**Monday Morning, June 17**

**Energetic Material Synthesis**

Discussant: Jeff Botaro (SRI)  
9:00-9:40 Mike Hiskey (LANL) Explosive Synthesis at Los Alamos National Laboratory  
10:00 Coffee & Photo  
10:30-11:10 Bob Chapman (NAWC) Energetic Potpourri  
11:30-12:10 Surya Prakash (USC) Studies on Potential Energetic Nitro Functional Groups & Compounds

**Monday 4:30-6:00; June 17**

**Poster Session "M" & Reception**

**Monday Evening, June 17**

**Energetic Material Synthesis**

Discussant: Phil Pagoria (LLNL)  
7:30-8:00 Ross Millar (DRA) Newer Nitration Methods for Synthesis of Energetic Compounds  
8:15-8:35 Mike Coburn (LANL) Synthesis & NMR of  $^2\text{H}$ ,  $^{13}\text{C}$ , and  $^{15}\text{N}$  Labeled Derivatives of TNAZ  
8:45-9:25 Alan Marchand (UNT) & Bob McKenney Synthesis of 1,3,3-Trinitroazetidine (TNAZ) & Related Compounds

**Tuesday Morning, June 18**

**Initiation and Detonation Models**

Discussant: Carl Melius (Sandia, CA)  
9:00-9:40 John Gilman (UCLA) Mechanochemistry at Detonation Fronts in Solids  
10:00 Coffee  
10:15-10:55 Joe Shepard (CalTech) What Kind of Chemistry Do You Have in Your Detonation?  
11:15-11:55 Barry Kunz (Michigan Tech) Excited Electronic States in Initiation of Solid Detonations  
12:10-12:30 Malcolm Nicol (UCLA) Some Thoughts on Initiation and Detonation Models

**Tuesday 4:30-6:00, Poster Session "T"**

**Tuesday Evening, June 18**

**Energetic Polymers**

Discussant: Tom Archibald (Aerojet)  
7:30-8:00 Lou Cannizzo (Thiokol) Effects of Chemical Structure on Physical Properties in Oxetane Polymers  
8:15-8:45 Gerry Manser (Aerojet) Development of Energetic Oxetane Polymers  
9:00-9:30 Don Thompson (Oklahoma S) Theoretical Chemical Dynamics Studies of Energetic Materials

**Wednesday Morning, June 19**

**Non-Ideal Explosives**

Discussant: Kevin McNesby (ARL)  
9:00 John Lee (McGill) On Modeling of the Rate Law for Non-Ideal Explosives  
10:00 Coffee  
10:30 Scott Stewart (U of Illinois) Ignition Mechanisms of Energetic Materials  
11:30-12:10 Jerry Forbes (NSWC) Detonation Properties of Non-ideal Explosives

**Wednesday Evening, June 19**  
**Experimental Examination of Detonation & Combustion**

Discussant: Randy Simpson (LLNL)  
7:30-8:10 Blaine Asay (LANL) Dynamic Measurement of Strain in Deforming of Explosives  
8:30-9:10 Ming-Chang Lin (Emory) Experimental & Theoretical Studies of Elementary Processes in Nitramine Combustion  
9:30-10:00 Joe Foster (Eglin) Mechanical Ignition of Combustion in Explosives

**Thursday Morning, June 20**

**Propellant Combustion**

Discussant: Tom Brill (U Delaware)  
9:00-9:40 Tom Litzinger (Penn State) Mass Spectroscopic Studies of Propellant Flames  
10:00 Coffee  
10:30-11:10 Vigor Yang (Penn State) Interaction between Unsteady Flow & Combustion of Energetic Materials  
11:30-12:10 Merrill Beckstead (BYU) Solid MonoPropellant Combustion

**Thursday Evening, June 20**

**Applied Explosives Chemistry**

Discussant: Mike McBride (Yale)  
7:30-8:10 Steve Burneister (FBI) The Forensics of Explosives  
8:30-9:10 Gerald Laib (NSWC) The Chemistry of Fireworks

# Conference Registration List

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