



CHEMICAL REACTIONS IN ENERGETIC MATERIALS¹

George F. Adams

Ballistic Research Laboratory, Aberdeen Proving Ground, Aberdeen,
Maryland 21005-5066

Robert W. Shaw, Jr.

Army Research Office, Research Triangle Park,
North Carolina 27709-2211

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INTRODUCTION

Energetic materials release energy as they transform from reactants to products. They have applications as explosives and rocket and gun propellants, in construction and mining, in emergency escape devices and automobile air bags, and in materials synthesis. Because large amounts of energy are released over a short period of time, investigation of these reactions poses a considerable challenge for the physical chemist. The development of the tools of physical chemistry during the past decade—fast laser and other optical diagnostic probes, powerful kinetic modeling, and accurate electronic structure and dynamics calculations—now make significant advances in our understanding possible. This review describes some of these advances.

We limit our discussion to topics on energetic materials that are of special interest to physical chemists—those experiments and calculations

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Chemical Dynamics Studies Of Reactions In Energetic Materials

**Donald L Thompson, Robert W
Shaw, Thomas B Brill**



Chemical Dynamics Studies Of Reactions In Energetic Materials:

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Richtlinien für die Überwachung von Wehrmachtangehörigen ausserhalb der geschlossenen Truppe und von Betreuungseinrichtungen in den Niederlanden ,1942 Chemical Dynamics Studies of Unimolecular Reactions in

Energetic Materials ,1997 Research performed over the period August 1 1992 to July 31 1996 supported by the U S Army Research Office Grant number DAAL03 92 G 0358 is described This research project was concerned with the development of methods and simulations to study the unimolecular reaction dynamics of polyatomic molecules of interest as energetic materials The research consisted of classical dynamics studies of the fundamental dynamics mode selectivity IVR in highly excited polyatomic molecules and simulations of unimolecular reactions Much of the effort was devoted to developing an improved potential energy surface to describe the unimolecular dissociation of RDX hexahydro 1 3 5 trinitro s triazine

Scientific and Technical Aerospace Reports ,1995 *Energetic Materials* ,2003-11-25 This volume provides an overview of current research and recent advances in the area of energetic materials focusing on decomposition crystal and molecular properties The contents and format reflect the fact that theory experiment and computation are closely linked in this field Since chemical decomposition is of fundamental importance in energetic performance this volume begins with a survey of the decomposition processes of a variety of energetic compounds This is followed by detailed studies of certain compounds and specific mechanisms such as nitro aci nitro tautomerism Chapter 6 covers the transition from decomposition to crystal properties with molecular dynamics being the primary analytical tool The next several chapters deal with different aspects of the crystalline state again moving from the general to particular There is also a discussion of methods for computing gas liquid and solid phase heats of formation Finally the last portion of this volume looks at the potential of high nitrogen molecules as energetic systems this has been of considerable interest in recent years Overall this volume illustrates the progress that has been made in the field of energetic materials and some of the areas of current activity It also indicates the challenges involved in characterizing and understanding the properties and behaviour of these compounds The work is a unique state of the art treatment of the subject written by pre eminent researchers in the field Overall emphasis is on theory and computation presented in the context of relevant experimental work Presents a unique state of the art treatment of the subject Contributors are preeminent researchers in the field **Overviews Of Recent Research On Energetic Materials**

Donald L Thompson,Robert W Shaw,Thomas B Brill,2005-08-02 Few books cover experimental and theoretical methods to characterize decomposition combustion and detonation of energetic materials This volume by internationally known and major contributors to the field is unique because it summarizes the most important recent work what we know with confidence and what main areas remain to be investigated Most chapters comprise summaries of work spanning decades and contain expert commentary available nowhere else Although energetic materials are its focus this book provides a guide to

modern methods for investigations of condensed and gas phase reactions Although these energetic reactions are complex and difficult to study the work discussed here provides readers with a substantial understanding of the behavior of materials now in use and a predictive capability for the development of new materials based on target properties *Chemistry and Physics of Energetic Materials* S.N. Bulusu,1990 Proceedings of the NATO Advanced Study Institute on Chemistry and Physics of the Molecular Processes in Energetic Materials Altavilla Milicia Sicily Italy September 3 15 1989 *AFOSR Chemical & Atmospheric Sciences Program Review* United States. Air Force. Directorate of Chemical and Atmospheric Sciences, **Research Interests of the Air Force Office of Scientific Research** ,1985 US Air Force Research Technology Area Plan ,1991

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Table of Contents Chemical Dynamics Studies Of Reactions In Energetic Materials

1. Understanding the eBook Chemical Dynamics Studies Of Reactions In Energetic Materials
 - The Rise of Digital Reading Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Advantages of eBooks Over Traditional Books
2. Identifying Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Chemical Dynamics Studies Of Reactions In Energetic Materials
 - User-Friendly Interface
4. Exploring eBook Recommendations from Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Personalized Recommendations
 - Chemical Dynamics Studies Of Reactions In Energetic Materials User Reviews and Ratings
 - Chemical Dynamics Studies Of Reactions In Energetic Materials and Bestseller Lists
5. Accessing Chemical Dynamics Studies Of Reactions In Energetic Materials Free and Paid eBooks
 - Chemical Dynamics Studies Of Reactions In Energetic Materials Public Domain eBooks
 - Chemical Dynamics Studies Of Reactions In Energetic Materials eBook Subscription Services

- Chemical Dynamics Studies Of Reactions In Energetic Materials Budget-Friendly Options
- 6. Navigating Chemical Dynamics Studies Of Reactions In Energetic Materials eBook Formats
 - ePub, PDF, MOBI, and More
 - Chemical Dynamics Studies Of Reactions In Energetic Materials Compatibility with Devices
 - Chemical Dynamics Studies Of Reactions In Energetic Materials Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Highlighting and Note-Taking Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Interactive Elements Chemical Dynamics Studies Of Reactions In Energetic Materials
- 8. Staying Engaged with Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Chemical Dynamics Studies Of Reactions In Energetic Materials
- 9. Balancing eBooks and Physical Books Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Chemical Dynamics Studies Of Reactions In Energetic Materials
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Setting Reading Goals Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Fact-Checking eBook Content of Chemical Dynamics Studies Of Reactions In Energetic Materials
 - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
- 14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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