



Chemical Dynamics Studies Of Reactions In Energetic Materials

Joacim Rocklöv



Chemical Dynamics Studies Of Reactions In Energetic Materials:

Richtlinien für die Überwachung von Wehrmachtangehörigen ausserhalb der geschlossenen Truppe und von Betreuungseinrichtungen in den Niederlanden ,1942 **Epistola Andraedis ad Curillum, ut in Pindum se recipiat, musasque defendat a malenatis Frisiæ poëtis** ,1746 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

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 *Scientific and Technical Aerospace Reports* ,1995 *Energetic Materials*

,2003-11-21 This volume provides an overview of current research and recent advances in the area of energetic materials focusing on explosives and propellants The contents and format reflect the fact that theory experiment and computation are closely linked in this field The challenge of developing energetic materials that are less sensitive to accidental stimuli continues to be of critical importance This volume opens with discussions of some determinants of sensitivity and its correlations with various molecular and crystal properties The next several chapters deal in considerable detail with different

aspects and mechanisms of the initiation of detonation and its quantitative description The second half of this volume focuses upon combustion Extensive studies model ignition and combustion with applications to different propellants The final chapter is an exhaustive computational treatment of the mechanism and kinetics of combustion initiation reactions of ammonium perchlorate 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 *Research Interests of the Air Force Office of Scientific Research* ,1991

Research in Progress United States. Army Research Office, 1992 Vols for 1977 consist of two parts Chemistry biological sciences engineering sciences metallurgy and materials science issued in the spring and Physics electronics mathematics geosciences issued in the fall US Air Force Research Technology Area Plan ,1991

Descriptive Summaries for Program Elements of the Research, Development, Test and Evaluation, Army Program, FY 1987 (U), February 1986 ,1986 **Energy Research Abstracts** ,1994 *AFOSR Chemical & Atmospheric Sciences Program Review* United States. Air Force. Directorate of Chemical and Atmospheric Sciences, Static Compression of Energetic Materials Suhithi M. Peiris, Gasper J. Piermarini, 2009-01-03 Developing and testing novel energetic materials is an expanding branch of the materials sciences Reaction detonation or explosion of such materials invariably produce extremely high pressures and temperatures To study the equations of state EOS of energetic materials in extreme regimes both shock and static high pressure studies are required The present volume is an introduction and review of theoretical experimental and numerical aspects of static compression of such materials Chapter 1 introduces the basic experimental tool the diamond anvil pressure cell and the observational techniques used with it such as optical microscopy infrared spectrometry and x ray diffraction Chapter 2 outlines the principles of high nitrogen energetic materials synthesis Chapters 3 and 4 examine and compare

various EOS formalisms and data fitting for crystalline and non crystalline materials respectively Chapter 5 details the reaction kinetics of detonating energetic materials Chapter 6 investigates the interplay between static and dynamic shock studies Finally Chapters 7 and 8 introduce numerical simulations molecular dynamics of energetic materials under either hydrostatic or uni axial stress and ab initio treatments of defects in crystalline materials This timely volume meets the growing demand for a state of the art introduction and review of the most relevant aspects of static compression of energetic materials and will be a valuable reference to researchers and scientists working in academic industrial and governmental research laboratories

Chemistry of Energetic Materials George A. Olah, David R. Squire, 2012-12-02 The study of energetic materials is emerging from one primarily directed toward practical interests to an advanced area of fundamental research where state of the art methods and theory are used side by side with modern synthetic methods This timely book integrates the recent experimental synthetic and theoretical research of energetic materials Editors George Olah and David Squire emphasize the importance of structure and mechanism in determining properties and performances They also explore new spectrometric methods and synthetic approaches in this useful reference Discusses structural analysis by x ray crystallography Explains chemical dynamics by photofragmentation translational spectroscopy Covers kinetic analysis by ultrafast absorption and emission spectroscopy Details syntheses of polycyclic caged amines fuel additives and polynitro compounds Examines computer aided design of monopropellants Includes contributions by two Nobel laureates and five members of the National Academy of Sciences

Chemistry and Physics of Energetic Materials S.N. Bulusu, 2012-12-06 This book represents a collection of lectures presented at the NATO Advanced study Institute ASI on Chemistry Physics of the Molecular Processes in Energetic Materials held at Hotel Torre Normanna Altavilla Milicia Sicily Italy September 3 to 15 1989 The institute was attended by seventy participants including twenty lecturers drawn from thirteen countries The purpose of the institute was to review the major advances made in recent years in the theoretical and experimental aspects of explosives and propellants In accordance with the format of the NATO ASI it was arranged to have a relatively small number of speakers to present in depth review type lectures emphasizing the basic research aspects of the subject over a two week period Most of the speakers gave two lectures each in excess of one hour with additional time for discussions The scope of the meeting was limited to molecular and spectroscopic studies since the hydrodynamic aspects of detonation and various performance criteria of energetic materials are often covered adequately in other international meetings An attempt was made to have a coherent presentation of various theoretical computational and spectroscopic approaches to help a better understanding of energetic materials from a molecular point of view The progress already made in these areas is such that structure property e g

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