

Unit –II : Chemical Dynamics

Potential energy surfaces, Kinetic isotopic effects - Dynamics of unimolecular reactions – Lindemann-Hinshelwood – Rice Ramsperger Kassel (RRK) theory and Rice Ramsperger Kassel – Marcus (RRKM) theory. Study of fast reactions by laser, relaxation, flash Photolysis and nuclear magnetic resonance methods. LFERs -Hammett equation, Taft equation, separation of polar, resonance and steric effects.

Chemical Dynamics Studies Of Unimolecular Reactions In Energetic Materials

Didier Mathieu



Chemical Dynamics Studies Of Unimolecular Reactions In Energetic Materials:

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

Chemical Dynamics Studies of Reactions in Energetic Materials, 1993 We have carried out a research program to investigate the chemical dynamics of unimolecular reactions in large polyatomic molecules The purpose of the studies is an improved understanding of the fundamental behavior of highly excited reactive molecules with an emphasis on energetic materials We have made some significant progress in extending theoretical chemical dynamics calculations to reactions in large molecules as illustrated by our explicit full dimensional classical dynamics study of the unimolecular decomposition of RDX Leading up to this study of RDX we performed a long series of dynamics calculations 2 30 for a variety of molecules to determine the important factors for accurately simulating processes in polyatomic molecules

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

Research in Progress, 1992 **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 Scientific and Technical Aerospace Reports ,1995 *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 **Molecular Modeling of the Sensitivities of Energetic Materials** Didier Mathieu,2022-04-05 Molecular Modeling of the Sensitivities of Energetic Materials Volume 22 introduces experimental aspects explores the relationships between sensitivity molecular structure and crystal structure discusses insights from numerical simulations and highlights applications of these approaches to the design of new materials Providing practical guidelines for implementing predictive models and their application to the search for new compounds this book is an authoritative guide to an exciting field of research that warrants a computer aided approach for the investigation and design of safe and powerful explosives or propellants Much recent effort has been put into modeling sensitivities with most work focusing on impact sensitivity and leading to a lot of experimental data in this area Models must therefore be developed to allow evaluation of significant properties from the structure of constitutive molecules Highlights a range of approaches for computational simulation and the importance of combining them to accurately understand or estimate different parameters Provides an overview of experimental findings and knowledge in a quick and accessible format Presents guidelines to implement sensitivity models using open source python related software thus supporting easy implementation of flexible models and allowing fast assessment of hypotheses Inventory of Energy Research and Development, 1973-1975 Oak Ridge National Laboratory,1976 Theoretical Studies of the Chemical Dynamics of Unimolecular Processes Donald L. Thompson,OKLAHOMA STATE UNIV STILLWATER DEPT OF CHEMISTRY.,1988 The purpose of this research program was to develop computational methods and carry out calculations to investigate the chemical dynamics of large molecules of interest as energetic materials Classical dynamics studies were made of the intramolecular vibrational energy redistribution and unimolecular reactions in a wide variety of polyatomic molecules including benzene toluene dimethylnitramine hydrogen peroxide HONO and methyl nitrite These studies are described in this report jes

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