

Cambridge University Press  
978-0-521-82819-2 - Dissociative Recombination of Molecular Ions  
Mats Larsson and Ann E. Orel  
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## DISSOCIATIVE RECOMBINATION OF MOLECULAR IONS

Dissociative recombination (DR) of molecular ions with electrons is a complex, poorly understood molecular process. Its critical role as a neutralizing agent in the Earth's upper atmosphere is now well established and its occurrence in many natural and laboratory produced plasmas has been a strong motivation for studying the event. For the first time, theoretical concepts, experimental methodology, and applications are united in one book, revealing the governing principles behind the gas-phase reaction. The book takes the reader through the intellectual challenges posed, describing in detail dissociation mechanisms, dynamics, diatomic and polyatomic ions, and related processes, including dissociative excitation, ionpair formation and photodissociation. With the final chapter dedicated to applications in astrophysics, atmospheric science, plasma physics, and fusion research, this is a focused, definitive guide to a fundamental molecular process. The book will appeal to academics within physics, physical chemistry, and related sciences.

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We would like to dedicate this book to Sheldon Datz, who was responsible for introducing us to this interesting area of physics.

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## Preface

This research monograph provides a single-volume description of the dissociative recombination of molecular ions with electrons. Since this is one of the most complex gas-phase processes, its study is a challenge to theorists and experimentalists alike. The theory, experiment, and applications of dissociative recombination are scattered in the scientific literature as original research articles, conference proceedings, and review articles. This book brings this information together in a single work for the first time.

The book is intended for researchers and Ph.D. students in the fields of atomic and molecular physics, chemical physics and physical chemistry, molecular astrophysics, atmospheric physics, and other areas of science where electrons and molecular ions are important.

This book was written during a period when each of us had several other commitments which slowed down the writing. One of us (AEO) was department chair at UC Davis essentially during the entire writing process, and ML chaired committees for the Swedish Space Board and the Swedish Research Council.

We are grateful for the hospitality of the Institute for Atomic and Molecular Physics (ITAMP) at the Harvard-Smithsonian Center for Astrophysics and Harvard University Physics Department (Kate Kirby, Hussein Sadeghpour), the Cluster Research Laboratory, Toyota Technological Institute, Tokyo (Tamotsu Kondow), and the University of Chicago (Takeshi Oka), all of which provided excellent working conditions for us when we needed to get away from our home institutions to focus on writing.

Several people have assisted us in reading part of the book and making valuable suggestions: Alex Dalgarno, Shirzad Kalhori, Holger Kreckel, Åsa Larson, Valery Ngassam, Takeshi Oka, Jeanna Royal, Albert Viggiano and Vitali Zhaunerchyk. We offer them our sincerest thanks for their help.

Finally we would like to thank Rainer Johnson, Brian Mitchell, Ioan Schneider, Andreas Wolf, Chris Greene, and the members of our research groups for access to material prior to publication.

Dissociative recombination of vibrationally relaxed  $\text{H}_2\text{O}^+$  ions with electrons has been studied in the heavy-ion storage ring CRYRING. Absolute cross-sections have been measured for collision energies between 0 eV and 30 eV. The energy dependence of the cross-section below 0.1 eV is found to be much steeper than the  $E^{-1}$  behaviour associated with the dominance of the direct recombination mechanism. Resonant structures found at 4 eV and 11 eV have been attributed to the electron capture to Rydberg states converging to electronically excited ionic states. Complete branching fractions for all dissociative recombination and rotational excitation are the potential energy curve (PEC) of the ground state of the ion, the PECs of the neutral valence dissociative states interacting with the ionization continua, those of the Rydberg states associated to these continua below the threshold (leading to smooth R-dependent quantum defects) and all the relevant Rydberg-valence. [13], given in Figures 3 and 4 of the same reference and are shown on the right side of Figure 1. Using this set of molecular data (PECs, electronic couplings and quantum defects), we performed a series of full rotational MQDT calculations of the cross sections for dissociative recombination for vibrationally relaxed  $\text{CH}^+$  molecular ions on their first 11 rotational levels. Cambridge University Press, 2008, 380 pages.

Dissociative recombination (DR) of molecular ions with electrons is a complex, poorly understood molecular process. Its critical role as a neutralising agent in the Earth's upper atmosphere is now well established and its occurrence in many natural and laboratory produced plasma has been a strong motivation for studying the event. For the first time, theoretical concepts, experimental methodology and applications are united in one book, revealing the governing principles behind the gas-phase reaction. Dissociative recombination is a process where a positive molecular ion recombines with an electron, and as a result, the neutral molecule dissociates. This reaction is important for extraterrestrial and atmospheric chemistry. On Earth, dissociative recombination rarely occurs naturally, as free electrons react with any molecule (even neutral molecules) they encounter. Even in the best laboratory conditions, dissociative recombination is hard to observe, but is an important reaction in systems that

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