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Theoretical Calculation of Ground and Electronically Excited States of MgRb^+ and SrRb^+ Molecular Ions: Electronic Structure and Prospects of Photo-Association

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Abstract

In this work, a comprehensive theoretical investigation is carried out to explore the electronic and spectroscopic properties of selected diatomic molecular ions MgRb^+ and SrRb^+ . Using high-level *ab initio* calculations based on a pseudopotential approach, along with large Gaussian basis sets and full valence configuration interaction (FCI), we accurately determine adiabatic potential energy curves, spectroscopic constants, transition dipole moments (TDMs), and permanent electric dipole moments (PDMs). To deepen our understanding of these systems, we calculate radiative lifetimes for vibrational levels in both ground and low-lying excited electronic states. This includes evaluating spontaneous and stimulated emission rates, as well as the effects of blackbody radiation. We also compute Franck–Condon factors and analyze photoassociation processes for both ions. Furthermore, to explore low-energy collisional dynamics, we investigate elastic scattering in the first excited states ($2^1\Sigma^+$) describing the collision between the Ra atom and Mg^+ or Sr^+ ions. Our findings provide detailed insights into the theoretical electronic structure of these molecular ions, paving the way for future experimental studies in the field of cold and ultracold molecular ion physics.

Keywords: *ab initio*; pseudopotential; configuration interaction; potential energy curves; spectroscopic constants; dipole moment; vibrational levels; elastic collision



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1. Introduction

Molecular ions formed through the interaction of trapped ions and ultracold atoms have recently attracted considerable attention as a promising candidate for investigating fundamental aspects of quantum-controlled chemistry, cold collision dynamics [1–7]. Their unique long-range interactions and controllable internal degrees of freedom make them highly suitable for a variety of applications. These include high-resolution molecular spectroscopy [2], ultracold collision studies [5–9], quantum computing [10,11], precision measurement [12], quantum simulation [11–15], and investigations into many-body physics [16]. A common experimental setup for ion–atom studies features laser-cooled alkaline-earth-metal ions confined in a Paul trap, overlapped with ultracold alkali-metal

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Photochemistry and Photophysics Vincenzo Balzani, Paola Ceroni, Alberto Juris, 2014-06-09 This textbook covers the spectrum from basic concepts of photochemistry and photophysics to selected examples of current applications and research. Clearly structured, the first part of the text discusses the formation, properties and reactivity of excited states of inorganic and organic molecules and supramolecular species as well as experimental techniques. The second part focuses on the photochemical and photophysical processes in nature and artificial systems using a wealth of examples taken from applications in nature, industry and current research fields ranging from natural photosynthesis to photomedicine, polymerizations, photoprotection of materials, holography, luminescence sensors, energy conversion and storage and sustainability issues. Written by an excellent author team combining scientific experience with didactical writing skills, this is the definitive answer to the needs of students, lecturers and researchers alike going into this interdisciplinary and fast growing field.

Scientific and Technical Aerospace Reports, 1976 Lists citations with abstracts for aerospace related reports obtained from world wide sources and announces documents that have recently been entered into the NASA Scientific and Technical Information Database.

Proceedings of the National Academy of Sciences of the United States of America National Academy of Sciences (U.S.), 1926 The Proceedings of the National Academy of Sciences (PNAS) publishes research reports, commentaries, reviews, colloquium papers and actions of the Academy. PNAS is a multidisciplinary journal that covers the biological, physical and social sciences.

Physical Review, 1929 Vols for 1903 include Proceedings of the American Physical Society.

Handbook of Molecular Physics and Quantum Chemistry, 3 Volume Set Stephen Wilson, 2003-03-07 Published in three volumes, this comprehensive reference work brings together in a single source for the first time a detailed presentation of the most important theoretical concepts and methods for the study of molecules and molecular systems. The logical format of the Handbook allows the reader to progress from the foundations of the field to the most important and exciting areas of current research. Edited and written by an outstanding international team and containing over 100 articles written by more than 50 contributors, it will be invaluable for both the expert researcher and the graduate student or postdoctoral worker active in any of the broad range of fields where these concepts and methods are important. Comprises three themed volumes: Fundamentals, Molecular Electronic Structure, Molecules in the Physico-Chemical Environment, Spectroscopy, Dynamics and Bulk Properties. Presents detailed articles covering the key topics presented in a didactic manner. Focuses both on theory and the relation of experiment to theory. Volume 1 Fundamentals presents the foundations of molecular physics and quantum chemistry. It consists of 7 parts arranged as follows: Part 1 Introduction, Part 2 Elements of Quantum Mechanics, Part 3 Orbital Models for Atomic, Molecular and Crystal Structure, Part 4 Symmetry Groups and Molecular Structure, Part 5 Second Quantization and Many Body Methods, Part 6 Approximate Separation of Electronic and Nuclear Motion, Part 7 Quantum Electrodynamics of Atoms and Molecules. The central problem of molecular physics and

quantum chemistry is the description of atomic and molecular electronic structure The development of appropriate models for the description of the effects of electron correlation and of relativity are key components of the analysis Volume 2 Molecular Electronic Structure addresses these topics and consists of 7 parts arranged as follows Part 1 Approximation methods Part 2 Orbital Models and Generalized Product Functions Part 3 Electron correlation Part 4 Relativistic molecular electronic structure Part 5 Electronic structure of large molecules Part 6 Computational quantum chemistry Part 7 Visualization and interpretation of molecular electronic structure In reality no molecular system exists in isolation Molecules interact with other atoms and molecules and with their environment Volume 3 Molecules in the Physico Chemical Environment Spectroscopy Dynamics and Bulk Properties consists of 7 parts arranged as follows Part 1 Response theory and propagator methods Part 2 Interactions between molecules Part 3 Molecules in different environments Part 4 Molecular Electronic spectra Part 5 Atomic Spectroscopy and Molecular Vibration Rotation Spectroscopy Part 6 Molecular dynamics and dynamical processes Part 7 Bulk properties

Annual Review Bunshi Kagaku Kenkyūjo,2006 **Russian Journal of Physical Chemistry** ,2002 **British Chemical Abstracts** ,1926 Bulletin of the Chemical Society of Japan Nihon Kagakkai,1999 **Proceedings of the 2nd International Workshop on Auger Spectroscopy and Electronic Structure (IWASES-II), Malmö, Sweden, September 4-6, 1991** Klaus Wandelt,C.-O. Almbladh,R. Nyholm,1992 Book of Abstracts American Chemical Society. Meeting,American Chemical Society,1987 *Soviet Physics, Uspekhi* ,1991 Optics and Spectroscopy ,2006 Il Nuovo Cimento Della Società Italiana Di Fisica ,1991 **The Journal of Chemical Physics** ,2003 **Physical Chemistry** Keith James Laidler,John H. Meiser,1995 After explaining the experimental and theoretical reasoning behind fundamental concepts of physical chemistry this text moves into a discussion of the concept itself This narrative approach which incorporates historical vignettes aims to give a greater understanding of the material and brief biographies of famous physical chemists are provided to help students to see how theories have developed and to add interest to the course Problems worked out examples and suggested readings are included *Conference Papers Index* ,1980 *The National Research Council Review* ,1965 Summaries of FY ... Research in the Chemical Sciences ,1995 **Kinetics and Catalysis** ,1977

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