

## Article

# Theoretical Calculation of Ground and Electronically Excited States of $\text{MgRb}^+$ and $\text{SrRb}^+$ 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  $\text{MgRb}^+$  and  $\text{SrRb}^+$ . 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 Rb atom and  $\text{Mg}^+$  or  $\text{Sr}^+$  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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## **Table of Contents Structure Of Electronically Excited Spec**

1. Understanding the eBook Structure Of Electronically Excited Spec
  - The Rise of Digital Reading Structure Of Electronically Excited Spec
  - Advantages of eBooks Over Traditional Books
2. Identifying Structure Of Electronically Excited Spec
  - 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 Structure Of Electronically Excited Spec
  - User-Friendly Interface
4. Exploring eBook Recommendations from Structure Of Electronically Excited Spec
  - Personalized Recommendations
  - Structure Of Electronically Excited Spec User Reviews and Ratings
  - Structure Of Electronically Excited Spec and Bestseller Lists
5. Accessing Structure Of Electronically Excited Spec Free and Paid eBooks
  - Structure Of Electronically Excited Spec Public Domain eBooks
  - Structure Of Electronically Excited Spec eBook Subscription Services
  - Structure Of Electronically Excited Spec Budget-Friendly Options
6. Navigating Structure Of Electronically Excited Spec eBook Formats

- ePub, PDF, MOBI, and More
- Structure Of Electronically Excited Spec Compatibility with Devices
- Structure Of Electronically Excited Spec Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Structure Of Electronically Excited Spec
  - Highlighting and Note-Taking Structure Of Electronically Excited Spec
  - Interactive Elements Structure Of Electronically Excited Spec
- 8. Staying Engaged with Structure Of Electronically Excited Spec
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Structure Of Electronically Excited Spec
- 9. Balancing eBooks and Physical Books Structure Of Electronically Excited Spec
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Structure Of Electronically Excited Spec
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Structure Of Electronically Excited Spec
  - Setting Reading Goals Structure Of Electronically Excited Spec
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Structure Of Electronically Excited Spec
  - Fact-Checking eBook Content of Structure Of Electronically Excited Spec
  - 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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