



Article

# Theoretical Calculation of Ground and Electronically Excited States of MgRb<sup>+</sup> and SrRb<sup>+</sup> 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<sup>+</sup> and SrRb<sup>+</sup>. 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 ( $2^1\text{E}^+$ ) describing the collision between the Ra atom and Mg<sup>+</sup> or Sr<sup>+</sup> 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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