

# An ab initio investigation on the low-lying electronic states of NaMg

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# **An *ab initio* investigation on the low-lying electronic states of NaMg**

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**Abstract:** Theoretical investigations for NaMg have been performed on the icMRCI+Q level employing basis set of quintuple- $\zeta$  quality with corrections of core-valence correlation and scalar relativistic effect. The geometrical parameters, potential energy curves, vibrational energy levels, spectroscopic constants for the eight  $\Lambda$ -S states, with respect to the lowest four dissociation limits, are investigated. Through the spin-orbit coupling effect, these states split into fourteen  $\Omega$  states. The permanent dipole moments, transition dipole moments, Einstein emission coefficients, radiative lifetimes and Franck-Condon factors for all  $\Omega$  states are studied. The feasibility of performing laser cooling of NaMg has also been discussed. Our predictive results are anticipated to serve as guidelines for further researches on NaMg.

**Keywords:** NaMg; *ab initio* calculations; electronic structure; spin-orbit couplings; spectroscopic constants

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