Theoretical Investigation of the BeRb2+, BeCs2+ and SrRb2+ Dications

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Abstract

In this theoretical study, we investigate the electronic potential energy curves, spectroscopic parameters, vibrational energy levels and transition dipole moments for the diatomic dications BeRb2+, BeCs2+ and SrRb2+. We consider an ab initio approach based on the use of non-empirical pseudopotentials and parameterized l dependent polarization potentials. Results show that 1-22Σ+ for BeRb2+, 1-52Σ+ for BeCs2+ and 1-32Σ+ for SrRb2+ are repulsive. While the 32Σ+ for BeRb2+, 42Σ+ for BeCs2+ and 42Σ+ for SrRb2+ are metastable states. These states can accommodate some vibrational energy levels. Interesting avoided crossings between some 2?+ states are localized and examined. Until now no experimental and theoretical studies have been made for each system. Consequently, we discuss our results by comparing with some data of similar systems. Besides, the transition dipole moments of the ground state to a few excited states are computed and presented. The information associated with the electronic structures, spectroscopic parameters as well as the transition properties that provide in this paper is anticipated to serve as guidelines for further experimental and theoretical researches for each diatomic dication considered in this work.

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