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Theoretical investigation on the low-lying electronic states of beryllium antimonide

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Abstract: The Λ -S electronic states with respect to the lowest four dissociation limits of BeSb are investigated theoretically on the icMRCI+Q level employing basis set of quintuple- ζ quality. The geometrical parameters, potential energy curves, vibrational energy levels, spectroscopic constants for the twelve Λ -S states are obtained, analyzed and compared with those of the Beryllium-VA group diatomic family species where data are available. The permanent dipole moments, transition dipole moments, Einstein emission coefficients, radiative lifetimes and Franck-Condon factors for interested Λ -S states are also derived. Further assessments of the spin-orbit coupling effect are performed for states associated with the first two dissociation asymptotes of BeSb. Four Λ -S states split into seven Ω states, and some of the PECs are distorted significantly through the spin-orbit coupling effect, which is similar to its isovalent diatomics BeAs. In consideration of potential risks of

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