Accepted Manuscript

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

Ning Wang, Ming-Jie Wan, Chuan-Zhao Zhang, Yuan-Yuan Jin, Wei-Bin Zhang, Shan-Jun Chen, Song Li

PII:	S1386-1425(18)30918-1
DOI:	doi:10.1016/j.saa.2018.09.056
Reference:	SAA 16497
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	13 July 2018
Revised date:	10 September 2018
Accepted date:	30 September 2018

Please cite this article as: Ning Wang, Ming-Jie Wan, Chuan-Zhao Zhang, Yuan-Yuan Jin, Wei-Bin Zhang, Shan-Jun Chen, Song Li , Theoretical investigation on the low-lying electronic states of beryllium antimonide. Saa (2018), doi:10.1016/j.saa.2018.09.056

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

Ning Wang[a], Ming-Jie Wan[b], Chuan-Zhao Zhang[a], Yuan-Yuan Jin[a], Wei-Bin Zhang[a], Shan-Jun Chen[a], Song Li[a,*]

[a] *School of Physics and Optoelectronic Engineering, Yangtze University, Jingzhou, China*

[b] *Computational Physics Key Laboratory of Sichuan Province, Yibin University, Yibin, China*

* Corresponding author: Dr. Song Li
School of Physics and Optoelectronic Engineering
Yangtze University
Nanhuan Road 1, Jingzhou
China
E-mail: lsong@yangtzeu.edu.cn
Tel: +86 716 8060942

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