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B. Ostojić, P. Schwerdtfeger, P.R. Bunker, Per Jensen

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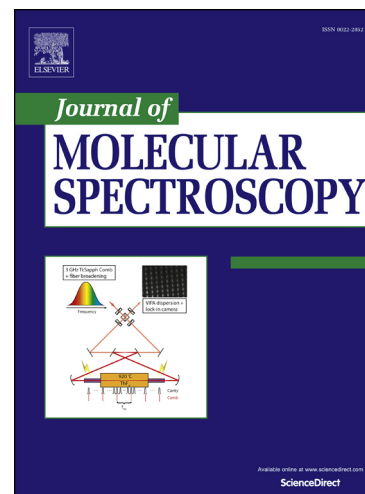
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An *ab initio* study of SbH₂ and BiH₂: The Renner Effect, Spin-Orbit Coupling, Local Mode Vibrations and Rovibronic Energy Level Clustering in SbH₂

B. Ostojić^a, P. Schwerdtfeger^b, P. R. Bunker^{b,1}, Per Jensen^{c,*}

^a*Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Studentski trg 14-16, 11 000 Belgrade, Serbia*

^b*Centre for Theoretical Chemistry and Physics (CTCP), The New Zealand Institute for Advanced Study(NZIAS), Massey University Auckland, Private Bag 102904, North Shore City, 0745 Auckland, New Zealand*

^c*Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Bergische Universität, D-42097 Wuppertal, Germany*

Abstract

We present the results of *ab initio* calculations for the lower electronic states of the Group 15 (pnictogen) dihydrides, SbH₂ and BiH₂. For each of these molecules the two lowest electronic states become degenerate at linearity and are therefore subject to the Renner effect. Spin-orbit coupling is also strong in these two heavy-element containing molecules. For the lowest two electronic states of SbH₂, we construct the three dimensional potential energy surfaces and corresponding dipole moment and transition moment surfaces by multi-reference configuration interaction techniques. Including both the Renner effect and spin-orbit coupling, we calculate term values and simulate the rovibrational and rovibronic spectra of SbH₂. Excellent agreement is obtained with the results of matrix isolation infrared spectroscopic studies and with gas phase electronic spectroscopic studies in absorption. For the heavier dihydride BiH₂ we calculate bending potential curves and the spin-orbit coupling constant for comparison. For SbH₂ we further study the local mode vibrational behavior and the formation of rovibronic energy

*Corresponding author.

Email address: jensen@uni-wuppertal.de (Per Jensen)

URL: <http://www.ptc.uni-wuppertal.de/jensen.html> (Per Jensen)

¹Permanent address: Steacie Laboratory, National Research Council of Canada, Ottawa, Ontario K1A0R6, Canada

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