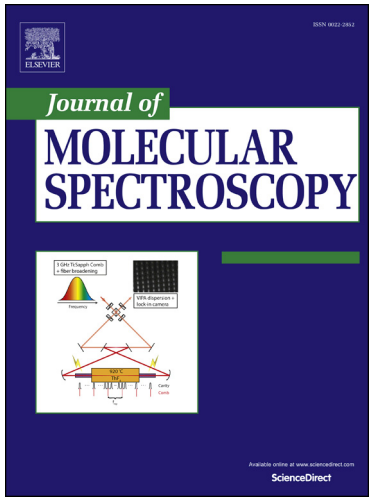

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B. Ostojić, P. Schwerdtfeger, P.R. Bunker, Per Jensen

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An *ab initio* study of SbH_2 and BiH_2: The Renner Effect, Spin-Orbit Coupling, Local Mode Vibrations and Rovibronic Energy Level Clustering in SbH_2

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, SbH_2 and BiH_2. 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 SbH_2, 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 SbH_2. 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 BiH_2 we calculate bending potential curves and the spin-orbit coupling constant for comparison. For SbH_2 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)

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