

AN *AB INITIO* STUDY OF  $\text{SbH}_2$  AND  $\text{BiH}_2$ : THE RENNER EFFECT, SPIN-ORBIT COUPLING, LOCAL MODE VIBRATIONS AND ROVIBRONIC ENERGY LEVEL CLUSTERING IN  $\text{SbH}_2$

BOJANA OSTOJIC, *Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Belgrade, Serbia*; PETER SCHWERDTFEGGER, *The New Zealand Institute for Advanced Study, Massey University, Auckland, New Zealand*; PHIL BUNKER, *Steacie Laboratory, National Research Council of Canada, Ottawa, ON, Canada*; PER JENSEN, *Faculty of Mathematics and Natural Sciences, University of Wuppertal, Wuppertal, Germany*.

We present the results of *ab initio* calculations for the lower electronic states of the Group 15 (pnictogen) dihydrides,  $\text{SbH}_2$  and  $\text{BiH}_2$ . 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  $\text{SbH}_2$ , 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  $\text{SbH}_2$ . Excellent agreement is obtained with the results of matrix isolation infrared spectroscopic studies and with gas phase electronic spectroscopic studies in absorption [1,2]. For the heavier dihydride  $\text{BiH}_2$  we calculate bending potential curves and the spin-orbit coupling constant for comparison. For  $\text{SbH}_2$  we further study the local mode vibrational behavior and the formation of rovibronic energy level clusters in high angular momentum states.

[1] X. Wang, P. F. Souter and L. Andrews, *J. Phys. Chem. A* 107, 4244-4249 (2003)

[2] N. Basco and K. K. Lee, *Spectroscopy Letters* 1, 13-15 (1968)