AN AB INITIO STUDY OF SbH₂ AND BiH₂: THE RENNER EFFECT, SPIN-ORBIT COUPLING, LOCAL MODE VIBRATIONS AND ROVIBRONIC ENERGY LEVEL CLUSTERING IN SbH₂

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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 [1,2]. 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 level clusters in high angular momentum states.