THE RENNER EFFECT IN THE $\widetilde{X}\ ^2A''$ AND $\widetilde{A}\ ^2A'$ ELECTONIC STATES OF HSO/HOS

ROMAN I. OVSYANNIKOV, *Institute of Applied Physics, Russian Academy of Science, Ulyanov Street 46, Nizhny Novgorod, Russia 603950, and Physical and Theoretical Chemistry, Faculty of Mathematics and Natural Sciences, University of Wuppertal, D-42097 Wuppertal, Germany*; PER JENSEN, *Physical and Theoretical Chemistry, Faculty of Mathematics and Natural Sciences, University of Wuppertal, D-42097 Wuppertal, Germany*; TSUNEO HIRANO, *Department of Chemistry, Faculty of Science, Ochanomizu University, 2-1-1 Otsuka, Bunkyo-ku, Tokyo 112-8610, Japan*.

We report a theoretical investigation of the $\widetilde{X}\ ^2A''$ and $\widetilde{A}\ ^2A'$ electronic states of HSO/HOS. Both electronic states have nonlinear equilibrium geometries and they correlate with a $^2\Pi$ state at linearity so that they exhibit the Renner effect. In highly excited bending states, there is tunneling between two minima (with the H nucleus bound to the O or S nucleus, respectively) separated by a potential energy barrier of 17224.3 cm^{-1}. The linear geometry H-O-S is accessible to the molecule; the corresponding barrier is 11877.3 cm^{-1}. However, the barrier to the H-S-O linear geometry is 34775.2 cm^{-1} and we take this geometry to be inaccesible to the molecule since at such a large potential energy, our potential energy surfaces are not well defined and an an accurate calculation of the rovibronic energies is not possible at the present time. So in practice we consider only a single Renner effect here, namely that at the H-O-S linear geometry. Three-dimensional potential energy surfaces for the $\widetilde{X}\ ^2A''$ and $\widetilde{A}\ ^2A'$ electronic states of HSO have been calculated *ab initio* by the MR-SDCI+Q/[aug-cc-pCVQZ (S, O), aug-cc-pVQZ (H)] method, and the global potential energy surfaces for the states have been constructed. These surfaces have been used, in conjunction with the computer program DR [Odaka *et al.*, J. Mol. Structure **795**, 14 (2006); Odaka *et al.*, J. Chem. Phys. **126**, 094301 (2007)], for calculating HSO/HOS rovibronic energies in the electronic states $\widetilde{X}\ ^2A''$ and $\widetilde{A}\ ^2A'$. The results and analysis of the *ab initio* calculations, the rovibronic energies obtained, and analyses of the wavefunction for selected states will be presented.