HIGH RESOLUTION INFRARED MEASUREMENTS ON HSOH

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We report the first high resolution infrared measurements on oxadisulfane, HSOH. The molecule is non planar with a simple skew chain structure analogues to the kin molecules hydrogenperoxide, HOOH, and hydrogendisulfane, HSSH.

In 2001 Behnke et al.[a] synthesized HSOH by flash vacuum pyrolysis of di-*tert*-butyl sulfoxide in amounts which are sufficient for gas phase detection. Winnewisser et al.[a] recorded the pure rotation-torsional spectra of HSOH in gas phase at high resolution using the Cologne Terahertz Spectrometer. The ground state molecular constants have been obtained with high accuracy.

Recently we extended our studies into the mid infrared region. We recorded spectra between 380 and 1400 cm^{-1} and between 1850 and 3800 cm^{-1} by using a Fourier transform spectrometer. We undoubtedly detected the O-H stretching vibration at about 3625.5 cm^{-1} and we assigned almost 1500 lines to this fundamental vibrational mode. According to the orientation of the vibrational dipole moment, HSOH displays strong *a*-type and *c*-type transitions in the spectrum of the O-H stretching mode but no *b*-type transitions.

We have used Pickett's program[b] to fit more than 1300 transitions by employing a Watson Hamiltonian in S reduction. The ground state constants were fixed to the values achieved from our microwave experiment. We obtained rotational constants A, B, C, D_J, D_{JK}, D_K, d_1, d_2, and H_J for the first vibrational exited state and determined the position of the band origin at 3625,49917(20) cm^{-1}.

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[a] G. Winnewisser, F. Lewen, S. Thorwirth, M. Behnke, J. Hahn, J. Gauss, E. Herbst, *J. Chem. Phys.* **9** (2003) 5501–5510

[b] H. Pickett, *J. Mol. Spectrosc.* **148** (1991) 371–377