

## EQUILIBRIUM STRUCTURE OF THE SIMPLE SKEW CHAIN MOLECULE HSOH

OLIVER BAUM, STEPHAN SCHLEMMER, THOMAS F. GIESEN, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; JÜRGEN GAUSS, *Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany*.

In this paper we present an empirical equilibrium structure of HSOH, which is either known as oxadisulfane or hydrogen thioperoxide. The molecule is non planar with a simple skew chain structure analogues to the kin molecules hydrogen-peroxide, HOOH, and hydrogen-disulfane, HSSH.

Gas-phase studies on oxadisulfane were long time hampered due to the problems of synthesizing the molecule. As recently as in 2001 Behnke<sup>a</sup> found a way to produce the molecule by pyrolysis of di-*tert*-butyl sulfoxide. The first high resolution gas-phase measurements on HSOH were presented in 2003 by Winnewisser *et al.*<sup>b</sup>. Beside the measurements on HSOH they were able to assign the spectrum of H<sup>34</sup>SOH in natural abundance. In 2003 Behnke *et al.*<sup>c</sup> also recorded the spectra perdeutero oxadisulfane, DSOD, which was produced in a discharge of D<sub>2</sub>S together with D<sub>2</sub>O. Recently Baum *et al.*<sup>d</sup> reported the first high resolution measurements on single deuterated oxadisulfane, HSOD. The molecule was synthesized in a rf-discharge of pure sulphur and HDO.

Based on these highly precise data from our measurements on HSOH, H<sup>34</sup>SOH, DSOD<sup>e</sup>, and HSOD we derived an empirical equilibrium structure of oxadisulfane. The equilibrium rotational constants  $A_e$ ,  $B_e$ , and  $C_e$  were obtained from  $A_0$ ,  $B_0$ , and  $C_0$  which were corrected by vibration-rotation interactions constants  $\alpha_r$  from high-level *ab initio* calculations. The derived bond lengths and angles agree very well with those from high level quantum chemical calculations.

---

<sup>a</sup>M. Behnke, *Ph.D. thesis*, Universität zu Köln (2001)

<sup>b</sup>G. Winnewisser, F. Lewen, S. Thorwirth, M. Behnke, J. Hahn, J. Gauss, E. Herbst, *J. Chem. Phys.* **9** (2003) 5501–5510

<sup>c</sup>M. Behnke, J. Suhr, S. Thorwirth, F. Lewen, H. Lichau, J. Hahn, J. Gauss, K. M. T. Yamada, G. Winnewisser, *J. Mol. Spectrosc.* **221** (2003) 121–126

<sup>d</sup>O. Baum, S. Esser, N. Gierse, S. Brünken, F. Lewen, J. Hahn, J. Gauss, S. Schlemmer, T. F. Giesen, *J. Mol. Struct.* (2006) (accepted)

<sup>e</sup>S. Brünken, M. Behnke, S. Thorwirth, K. M. T. Yamada, T. F. Giesen, F. Lewen, J. Hahn, G. Winnewisser, *J. Mol. Struct.* **742** (2005) 237–242