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[a] 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.*[b]. Beside the measurements on HSOH they were able to assign the spectrum of $H^{34}SOH$ in natural abundance. In 2003 Behnke *et al.*[c] also recorded the spectra perdeutero oxadisulfane, DSOD, which was produced in a discharge of D_2S together with D_2O. Recently Baum et al.[d] 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, $H^{34}SOH$, DSOD[e], 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 α_r from high-level *ab initio* calculations. The derived bond lengths and angles agree very well with those from high level quantum chemical calculations.

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