

Abstract

In the scope of this thesis different traits of the elusive species HSOH have been examined. HSOH, either known as oxadisulfane or hydrogen thio-peroxide is the link between the well known molecules HSSH, disulfane, and HOOH, hydrogen peroxide. HSOH is not only interesting because of its relevance in the combustion theory of sulfur, the sulfur cycle in the atmosphere, or as possible constituent in the interstellar medium but also because of its substantially spectroscopical importance.

With two different rotor moieties, SH and OH, HSOH represents the most general case of a four-atomic, internally rotating chain molecule. In order to provide further improvement of the theoretical understanding of internal rotation earlier experimental studies by Winnewisser *et al.*¹ have been extended into the THz-region.

The first gas-phase detection of the singly deuterated oxadisulfane HSOD presented here provided the last piece of the puzzle to determine a semi-experimental equilibrium structure of HSOH.

In order to get information on the dynamics involved in the molecule, the measurements have been extended into the infrared region and both high frequency bond stretching modes $\nu_{OH} = 1$ and $\nu_{SH} = 1$ have been assigned. The analysis of the bands proves HSOH to be a fairly rigid “textbook” molecule in case of the OH-stretching mode, while the $\nu_{SH} = 1$ state shows a strong potential coupling to some dark state.

Last but not least, it turned out that HSOH exhibits an anomalous intensity pattern for rotational transitions involving $K_a > 3$ states. Even though this effect is not reported yet it seems to be not a special trait of HSOH, but rather a spectroscopic effect of general importance.

¹G. Winnewisser, F. Lewen, S. Thorwirth, M. Behnke, J. Hahn, J. Gauss, E. Herbst. Gas-Phase detection of HSOH: Synthesis by Flash Vacuum Pyrolysis of di-*tert*-butyl-sulfoxide and rotational-torsional spectrum. *Chem. Eur. J.* **9** (2003) 5501–5510.