THE ROTATIONAL SPECTRUM OF *CIS*- AND *TRANS*-HSSOH

MONIKA KOERBER, OLIVER BAUM, THOMAS F. GIESEN, and STEPHAN SCHLEMMER,
I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany.

In this talk we present the first pure rotational lines of Oxatrisulfane, HSSOH. Oxatrisulfane is one link between the well-known skew chain molecules HSSSH and HOOOH. The structure of trisulfane HSSSH has been determined using rotational spectroscopy by Liedke *et al.*[a] showing HSSSH to form two stable conformers, *trans* and *cis*, with the *trans*-conformer to be slightly more stable. Only recently hydrogen-trioxide HOOOH has been discovered by Suma *et al.*[b] observing the rotational spectra of the *trans* conformer. For this molecule no evidence for the *cis* structure has been found.

First experimental evidence for the formation of HSSOH was given by Königshofen *et al.*[c] via flash vacuum pyrolysis of t-BuS(O)St-Bu at T $> 700^{\circ}$C using IR-spectroscopy to monitor the pyrolysis products. We employed this method to synthesize HSSOH and performed first high-resolution millimeterwave measurements in the range of 75–120 GHz by introducing an all solid state spectrometer. More than 170 lines of the *cis* conformer and more than 30 lines of *trans*-HSSOH have been undoubtly identified. Both conformeres are close to the limiting case of a prolate symmetric top with $\kappa_{cis} = -0.925$ and $\kappa_{trans} = -0.924$ respectively. Their permanent dipole moment points mainly along the *b*- and *c*- principle axes and therefore the spectrum displays a clear perpendicular structure. For analyzing the identified lines a standard *S*-reduced Hamiltonian has been used and we were able to fit the rotational parameters A, B, C as well as the centrifugal distortion parameters D_J, D_{JK}, D_K, d_1 and d_2. The *c*-type transitions of *cis*-HSSOH are approx. 14 times more intense than the corresponding *b*-type transitions, whereas in case of *trans*-HSSOH the intensities of the *b*- and *c*-type transitions are almost equal. All experimentally derived parameters are in excellent agreement with those obtained by high level ab initio calculations[d].

[a] Liedtke *et al.*, *J. Mol. Struct.* **413** 265–270 (1997)
[b] Suma *et al.*, *JACS* **127** 14998–14999 (2005)
[c] Königshofen *et al.*, *Z. Anorg. Allg. Chem.* **625** 1779–1786 (1999)
[d] J. Gauss, private communication