ETHYLENE GLYCOL REVISITED - THE QUEST FOR HIGHER PRECISION

DINES CHRISTEN, *Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, D-72076 Tübingen, Germany*; L. H. COUDERT, *Laboratoire de Photophysique Moléculaire, CNRS, Bâtiment 210, Université de Paris Sud, F-91405 Orsay Cedex, France*; H. S. P. MÜLLER, *I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany*.

The rotation-tunneling spectra of the g'Ga and g'Gg conformers of ethylene glycol have been studied between 54 and 347 GHz by conventional absorption spectroscopy in order to unambigously assign transitions with high J- and K_a- quantum numbers and thus enhance the accuracy of the describing parameters as well as the predictive power of the model for this very rich microwave spectrum. The current investigations were guided by fits and predictions based on a Reduced Axis System (RAS) Hamiltonian[a]. This is in contrast to the original investigations[b], where the spectra were modelled by an IAM-type Hamiltonian especially constructed for this problem.
Despite considerable Coriolis interaction between the two tunneling states of each conformer, more than 400 transitions of each conformer have been observed recently, including several x-type transitions. For the lower g'Ga conformer, transitions with J and K_a quantum numbers as high as 51 and 25, repectively, could be fit within experimental uncertainties with only 34 spectroscopic parameters: Rotational, quartic and sextic centrifugal constants for the 0^+ state, and changes of these constants for the 0^- state, along with eleven terms describing the Coriolis interaction between the 0^+- and 0^- states.
The investigations of the g'Gg conformer are not yet complete, but the present results suggest that with a similar parameter set eventually a comparably extensive data set will be fit within experimental accuracy.

[a] H. Pickett, *J. Chem. Phys.* **56** 1972, 1715.

[b] D. Christen, L. H. Coudert, R. Suenram and F. Lovas, *J. Mol. Spectrosc.* **172** 1995, 57-77. and D. Christen, L. H. Coudert, J. A. Larsson and D. Cremer, *J. Mol. Spectrosc.* **205** 2001, 185-196.