MILLIMETER AND SUBMILLIMETER WAVE SPECTROSCOPIC INVESTIGATIONS INTO THE ROTATION-TUNNELING SPECTRUM OF *gGg'* ETHYLENE GLYCOL ($HOCH_2CH_2OH$)

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Gaseous ethylene glycol (1,2-ethanediol) consists of two conformers, *aGg'* and *gGg'*, with the latter being $\sim 2.5\,\mathrm{kJ\,mol^{-1}}$ or $\sim 200\,\mathrm{cm^{-1}}$ higher in energy than the former. Both conformers exhibit intermolecular hydrogen bonding between the H atom of one OH group and the O atom of the other. Large amplitude tunneling occurs between two equivalent minima described by exchange of the roles of the H atoms of the OH groups. The two tunneling substates are separated by 6958 and 1367 MHz for *aGg'* and *gGg'* glycol, respectively, with considerable Coriolis interaction between the two substates.

Recently,[a] we have reported investigations into the rotation-tunneling spectrum of the *aGg'* conformer in selected regions between 54 and 370 GHz. The spectrum could be reproduced within experimental uncertainties employing a comparatively small set of spectroscopic parameters.

The present contribution deals with the rotation-tunneling spectrum of *gGg'* glycol recorded in selected regions between 77 and 579 GHz. While the quantum number range, $J \leq 55$ and $K_a \leq 19$, is similar to that of the *aGg'* study, a much larger number of transitions has been recorded because of persistent difficulties in reproducing the complete data set within experimental uncertainties. Starting to refit the transition frequencies involving low quantum numbers, it was possible to extend the line list in a consistent way to about 2/3 of the ~ 1500 transitions, i. e. to quantum numbers having $J \leq 40$ and $K_a \leq 4$ or $J \leq 22$ and $K_a \leq 17$ which could be reproduced within experimental uncertainties. Difficulties in fitting transitions with high J or K_a may be due to extensive Coriolis interaction between the two tunneling substates combined with unavoidable correlation effects or possibly to a Coriolis interaction of the ground vibrational state of *gGg'* glycol with the first excited torsional state of *aGg'* glycol.

[a] D. Christen and H. S. P. Müller, *Phys. Chem. Chem. Phys.* **5,** (2003) 3600–3605