

THE ROTATIONAL/CONCERTED TORSIONAL SPECTRUM OF THE g'Gg-CONFORMER OF ETHYLENE GLYCOL

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The microwave spectrum of the energetically unfavoured g'Gg-conformer of ethylene glycol is reported. This spectrum is dominated by an interconversion geared-type large amplitude motion during which each OH-group in turn forms the intramolecular hydrogen bond. The microwave spectrum has been analyzed using a Watson-type Hamiltonian plus a 1.4 GHz tunneling splitting. The rotational dependence of this tunneling splitting was examined using an IAM approach yielding quantitative information on the tunneling path between configurations. Unexpectedly, but in agreement with the ab initio calculations, both OH-groups are rotated through 240° in going from one equilibrium configuration to the other one, passing on the way through the g'Ga-conformations.