ROTATIONAL SPECTROSCOPY AND STRUCTURE OF THE GLYCIDOL-WATER HYDROGEN-BONDED COMPLEX

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Glycidol, also known as oxiranemethanol, is known to exist in two different conformational structures with different intramolecular hydrogen bonds from the alcohol to the oxirane oxygen. [a] [b] We have recorded 22 $a-$ and $b-$type rotational transitions of the glycidol-water complex; the rotational constants of the complex were determined to be A = 3902.331 MHz, B = 2763.176 MHz, and C = 1966.863 MHz by fitting to the Watson A-reduction Hamiltonian. The moment-of-inertia data was used to fit the structure of the glycidol-water complex. Water was found to insert itself into the hydrogen bonding network of the monomer, making a new network: alcohol to water oxygen and water to oxirane oxygen. MP2/6-311G** ab initio calculations were also used to model the structure and determine the relative conformer energies.

[a] W. V. F. Brooks and K. V. L. N. Sastry, Can. J. Chem. 53, 2247 (1975)

[b] K. -M. Marstokk, H. Møllendal, Y. Stenstrøm, Acta Chem. Scand. 46, 432 (1992).