THE MILLIMETER-WAVE ROTATIONAL SPECTRUM OF LACTIC ACID

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Lactic acid, $CH_3CH(OH)COOH$ ($C_3H_6O_3$) is a well-known molecule of biological relevance, and its basic properties are thus of fundamental interest. With molecular size at 12 atoms lactic acid falls somewhat outside the range of asymmetric-rotor molecules currently of interest in radioastronomy. It might, however, still be useful to consider it in checks run on available interstellar spectra, even if not as a direct search candidate. The rotational spectrum of lactic acid has previously been investigated at 28-38 GHz,^{*a*} resulting in assignment of the ground state and three vibrationally excited states.

Presently we report the results of a comprehensive investigation of the millimetre-wave rotational spectrum of lactic acid, over the region 160-320 GHz. Some measurements for the ground state were also made with supersonic expansion FTMW spectroscopy at 8-16 GHz. Octic level spectroscopic constants are reported for the ground state and many vibrationally excited states, which involve three different normal modes. Unambiguous vibrational assignment was possible on the basis of relative intensities and *ab initio* inertial defect calculations. The derived constants allow confident prediction of the rotational spectrum of lactic acid well into the sub-millimeter region. This work is also a first step in the investigation of the geometry, dipole moment and complexation of this molecule, currently in progress in our laboratory.

^aB.P. van Eijck, J.Mol.Spectrosc. 101, 133 (1983)