NEW MICROWAVE SPECTRUM AND GLOBAL FIT OF METHYL ACETATE GROUND STATE

I. KLEINER, M. TUDORIE, *Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris 7 et Paris 12, 61 av. Général de Gaulle, 94010, Créteil, France*; J. T. HOUGEN, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441, USA*; S. MELANDRI, *Dipartimento di Chimica "G.Ciamician", via Selmi 2, 40126 Bologna, Italy*; W. STAHL, L. SUTIKDJA, *Institut für Physikalische Chemie, Raum 234, RWTH Aachen, Landoltweg 2 52062 Aachen.*

Last year, we presented a newly written program to calculate and fit torsion-rotation transitions in molecules containing two inequivalent C_{3v} methyl tops and a plane of symmetry, based on the Hamiltonian described by Ohashi et al.[a], which in turn was based on earlier theoretical models cited in their references. We applied this code to refit microwave data for the methyl acetate molecule published in 1980[b]. Two sets of new measurements for this molecule were obtained, one using the Fourier transform microwave (FTMW) instrument in Aachen (4-18 GHz) with a measurement uncertainty of 5 kHz, the other using the millimeter wave (MMW) instrument in Bologna, (60-150 GHz) with a measurement uncertainty of 50 kHz. In the absence of top-top interactions, each asymmetric-top energy level splits into AA, AE, EA and EE components where the individual letters A and E indicate the symmetry species of the wave function with respect to internal rotation of one of the methyl tops. The new data for methyl acetate were assigned up to J=10 and put in the program. For the moment, almost all the 50 kHz measurements fit to experimental error, but we are still having trouble with the FTMW lines, which only fit to 7 kHz. By the time of the conference we hope to have found a better set of parameters, i.e., a set that describes more precisely the physical couplings occurring in this molecule[c].

[a] N. Ohashi, J. T. Hougen, R. D. Suenram, F.J. Lovas, Y. Kawashima, M. Fujitake and J. Pyka, J. Mol. Spectrosc., 227, 28-42 (2004)

[b] J. Sheridan, W. Bossert and A. Bauder, J. Mol. Spectrosc., 80, 1-11 (1980)

[c] Project partly supported by the ANR-08-BLAN-0054 contract (France)