MICROWAVE AND MILLIMETER WAVE SPECTRUM OF ACETIC ACID

I. KLEINER, Laboratoire de Photophysique Moléculaire, Université Paris Sud, 91405 Orsay Cédex, France; L. MARGULES, J. DEMAISON, G. WLODARCZAK and J. COSLEOU, Laboratoire de Spectroscopie Hertzienne, URA CNRS 249, Université Lille1, 59655 Villeneuve d’Ascq, France.

The microwave spectra of acetic acid (CH$_3$COOH) is complicated by a rather low internal rotation barrier of about 170 cm$^{-1}$, leading to A-E splittings sometimes as big as a few gigahertz. In spite of its astrophysical interest (acetic acid was detected recently in the Sgr B2 interstellar source$^a$ using millimeter arrays), the millimeter and microwave spectra of this molecule is far from being understood, especially in the torsional excited states. No really satisfactory agreement between observed and calculated frequencies was obtained up to now. Using data from the literature$^{b-f}$ and some new measurements performed with the Lille millimeter wave spectrometer, we began to apply the same RAM (Rho Axis Method) theoretical approach that we used successfully for a similar (from the internal rotation point of view) molecule, acetaldehyde CH$_3$CHO. Preliminary results involving the two first torsional states, $v_t=0$ and $v_t=1$ will be discussed.