MICROWAVE SPECTROSCOPY OF 2-FURANCARBOXYLIC ACID

R. MOTIYENKO[a], M. GOUBET, L. MARGULÈS, G. WLODARCZAK, *Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d'Ascq Cedex, France*; E. A. ALEKSEEV, S. F. DYUBKO, *Institute of Radio Astronomy of NASU, Chervonopraporna 4, 61002 Kharkov, Ukraine*.

The structure and harmonic force field of 2-furancarboxylic acid have been optimized at MP2/aug-cc-pVTZ level of theory. Geometries of four different conformations have been calculated: *Cc*, *Ct*, *Tc*, *Tt*. Two of them: *Cc* and *Tc* were unambiguously found the most stable conformations and very close in energy. Since two other conformers were found to be too high in energy (ΔE=9 kJ/mol and 23.5 kJ/mol correspondingly for *Tt* and *Ct*) only *Cc* and *Tc* conformations were considered in interpretation of the spectroscopic observations. The rotational spectra have been recorded in the frequency range 5 – 20 GHz using MB-MWFT spectrometer in Lille and in the frequency range 50 – 240 GHz using conventional absorption spectrometers in Kharkov and Lille. Rotational transitions of both *Cc* and *Tc* conformation have been assigned and rotational parameters have been obtained. It is interesting to note that for both conformations the values of sextic centrifugal distortion parameters were found to be too small and the rotational transitions with quantum number J as high as 80 and K_a as high as 50 can be fitted within experimental accuracy (0.010 – 0.020 MHz) using only quartic centrifugal distortion terms. Besides ground states several excited vibrational states have been assigned in conventional absorption spectra. Most of the excited states assigned were found to be coupled by Coriolis-type interaction. The results of microwave studies and ab initio calculations will be discussed.

[a]The support of INTAS YSF (INTAS Ref. Nr 06-1000014-5984) is gratefully acknowledged