FOURIER TRANFORM MICROWAVE STUDIES OF BI-MOLECULES OF CARBOXYLIC ACIDS

LUCA EVANGELISTI, GANG FENG, GOU QIAN, ASSIMO MARIS and W. CAMINATI, *Dipartimento di Chimica "G. Ciamician" dell'Università, Via Selmi 2, I-40126 Bologna, Italy*; LAURA B. FAVERO, *Istituto per lo Studio dei Materiali Nanostrutturati (ISMN, Sezione di Bologna), CNR, Via Gobetti 101, I-40129 Bologna, Italy*; EMILIO COCINERO, PATRICIA EJICA, JOSE' A. FERNANDEZ and FERNANDO CASTANO, *Departamento de Quimica Fisica, Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco, E-48080 Bilbao, Spain*; ALBERTO LESARRI, *Departamento de Quimica Fisica y Quimica Inorganica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain*; ROLF MEYER, *Sonnenbergstrasse 18, CH-5621 Zufikon, Switzerland*.

We recorded the molecular beam Fourier transform microwave spectra of several isotopic species of several homo and hetero dimers of carboxylic acids (R-COOH). Several tunnelling splittings have been measured with the accuracy underlying microwave spectroscopy. These splittings have been originated by the concerted double proton transfer of the two protons, but in some cases also by internal motions within the R chain in R-COOH. When the splittings were due to the double proton transfer, they were considerably decreasing upon mono- or bi-deuteration of the two carboxylic protons. The splittings due to the proton transfer have been used to determine the barrier to the proton transfer by applying a flexible model suited to take into account the coupling of the proton motions with the skeletal motions. The potential energy surfaces of the lateral chain motions have also been estimated. A full frame structure has been determined for some bimolecules, obtaining details of the Ubbelohde effect associated to the double hydrogen bond.