

FOURIER TRANSFORM MICROWAVE STUDIES OF BI-MOLECULES OF CARBOXYLIC ACIDS

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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.