Concerted proton transfer and conformational equilibria in bi-molecules of carboxylic acids

Walther Caminati[a], Luca Evangelisti[a], Gang Feng[a], Qian Gou[a], Assimo Maris, [a]
Laura B. Favero[b], Emilio Cocinero[c], Patricia Ejica[c], Fernando Castaño[c],
Alberto Lesarri[d], and Rolf Meyer[e]

[a] Dipartimento di Chimica "G. Ciamician" dell'Universita', Via Selmi 2, I-40126 Bologna, Italy, Ph: +390512099480; Fax: +390512099456; Email: walther.caminati@unibo.it.
[b] Istituto per lo Studio dei Materiali Nanostrutturati (ISMN, Sezione di Bologna), CNR, Via Gobetti 101, I-40129 Bologna, Italy; Ph: +390516399216; Email: L.Favero@bo.ismn.cnr.it.
[c] Departamento de Quimica Fisica, Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco, E-48080 Bilbao, Spain; Ph: +349460153870; Email: emiliojose.cocinero@ehu.es.
[d] Departamento de Quimica Fisica y Quimica Inorganica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain; Ph: +34983423206; Email: lesarri@qf.uva.es.
[e] Sonnenbergstrasse 18, CH-5621 Zufikon, Switzerland; Email: rolf.p.e.meyer@gmail.com.

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 bi-molecules, obtaining details of the Ubbelohde effect associated to the double hydrogen bond.