THE CIS-TRANS HYDROGEN BONDS IN β-PROPIOLACTONE$\cdots$HCl COMPLEX: A ROTATIONAL STUDY

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The rotational spectra of the hydrogen-bonded complex β-propiolactone$\cdots$HCl have been investigated using a molecular beam Fourier transform microwave spectrometer[a] equipped with a dual flow valve.[b] β-propiolactone ($C_3H_4O_2$) is a four-membered lactone ring which contain two oxygen atoms and may form three different 1:1 complexes with HCl. In the present work, only two of such complexes have been observed and characterized. In both cases the HCl subunit lies in the β-propiolactone ring plane and is bonded to the carbonyl group oxygen atom lone pairs in *cis* and *trans* positions with respect to the endocyclic lactone oxygen atom. The most stable *trans* form, observed using Ar and He as carrier gases, is stabilized by a bifurcated weak interaction of the Cl atom with the nearest ring methylene group hydrogen atoms. This interaction gives rise to a non linear arrangement of the O$\cdots$H–Cl fragment. The less stable *cis* form, only observed using He as carrier gas, has a linear arrangement of the atoms involved in the hydrogen bond and its structure reflects the effects of repulsive interactions between the Cl atom and the endocyclic oxygen atom of β-propiolactone. No signs of the conformer in which HCl is forming a hydrogen bond to this endocyclic oxygen atom have been observed in the supersonic jet. Considering that the HCl subunit acts as a probe of the electronic density regions on the proton acceptor molecule, the results of this study show that in lactones the highest nucelofility is associated to the carbonyl group oxygen atom.

[a] J. L. Alonso, F. Lorenzo, J. C. López, A. Lesarri, S. Mata and H. Dreizler; *Chem. Phys.*, **218**, 267 (1997).
[b] S. Antolínez, J. C. López, J. L. Alonso, *Chem. Phys. Letters*, **334**, 250 (2001).