

## Determining the Positions of Aromatic Hydrogens in (ar)C-H...X (X = O or F) Hydrogen Bonded Assemblies of Phenyl-phenyl, Phenyl-furyl Substituted Propenoic Acids and Esters from Their FTIR Spectra

I. Pálinkó<sup>1</sup>, J. Mink<sup>2,3</sup>

<sup>1</sup>Department of Organic Chemistry, University of Szeged, Dóm tér 8, Szeged, H-6720 Hungary

<sup>2</sup>Institute of Structural Chemistry, Chemical Research Center of the Hungarian Academy of Sciences, PoBox 17, Budapest H-1525 Hungary

<sup>3</sup>Faculty of Information Technology, Research Institute of Chemical and Process Engineering, University of Pannonia, Egyetem u. 10, Veszprém H-8200 Hungary

In the last couple of years the structure forming properties of various cinnamic acid and ester derivatives have been studied mostly with the combination of spectroscopic (mainly IR spectroscopy was applied) and computational methods (PM3 semiempirical method was used chiefly; originally the available computer power imposed us to use this level of theory, later the studied structures were extended to the size when this method could only be used even with increased computer power). As work went on even though the core structure was kept (propenoic acid that is), but the family of molecules has been largely extended. Phenyl (with occasionally, methoxy substituents) [1-3] and furyl [4] substituents were built into the unsaturated acid or methyl ester structure and, occasionally, the olefinic proton was also substituted for CF<sub>3</sub> group [5]. It has been found that short-range ordering (it was found in solutions) was originated in strong O-H...O hydrogen bonds for the acids, while weak (aromatic) C-H...O hydrogen bonds were responsible for long-range ordering only found in the solid state for the acids as well as the esters. These observations could be unequivocally stated, however, designating the positions of aromatic protons has not been attempted. Since in the meantime the variety of structures has been increased considerably enough data have been accumulated to assign now the aromatic protons to positions on the phenyl ring. This assignation is reported in this contribution.

The aggregating properties of a large variety of compounds have been studied. They were 2,3-phenyl or methoxy-substituted phenyl groups, 2,3-phenyl groups and a CF<sub>3</sub> group in position 3, 3,2-phenyl and furyl- substituted derivatives (acids as well as esters). Since each molecule contained at least one phenyl group collecting the normal modes of the phenyl groups was the first step. From this first step the assignment of vibrations to the protons in various positions followed. Fortunately, the bands belonging to the different (ar)C-H stretching vibrations could be separated in most cases, and thus, the work could be done.

The shifts in the relevant C-H stretching vibrations and the distances between the pillar atoms of the corresponding (aromatic)C-H...X hydrogen bonds have also been correlated.

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