Hydrogen Bonding Study by X-ray Difracction of Sugars and Aminoacids

María Dolores Estrada, M. Jesús Diánez, Amparo López-Catro, Simeón Pérez-Garrido, *Instituto de Ciencias de Materiales de Sevilla and Departamento de Física de la Materia Condensada C.S.I.C. Universidad de Sevilla Apdo. Correos 1065, E-4107.1 Seville, Spain.*
E-mail: estrada@us.es

The aim of this work is to study the different types of hydrogen bondings, by X-ray diffraction at room and low temperature, in biologically active molecules such as carbohydrates and aminoacids.

The effort will be mostly focused on sulfonic acids and their derivatives as they are important constituents of living organism found in nature as taurine (2-aminoethanesulfonic acid), homotaurine (3-aminopropanesulfonic acid), cysteic acid or guanidotaurine, and on structurally related sulfoamino carbohydrates and sulfoaminopoliols. All of them posses physiological properties essential for the well-being of various species. Taurine is present in relatively high concentration in the central nervous system and brain, acts as neurotransmitter in retine, and shows cardioprotective activity.

These compounds show zwitterion structure, with electrostatic and hydrogen bonding interaction between the protonated aminogroups and the sulfonate groups, that have been scarcely studied in solid state.

Cooperative hydrogen bonding, three- and four-center hydrogen bonds, and the role of the water molecules in the crystal stability, will be subject of a special study.

The study also involves the structural analysis of these compounds, to stablish their conformational and configurational characteristic unequivocally.

Keywords: sulfonic acids, hydrogen bonds, zwitterions