Charge Density of Amino Acids with Strong Hydrogen Bonds: A Comparative Study

Stefan Mebs[a], Christian Hübschle[a], Peter Luger[a], [a]*Institute of Chemistry/Crystallography, Free University of Berlin.* E-mail: stebs@chemie.fu-berlin.de

Submolecular electronic properties of functional groups in natural products are of particular interest for the pharmaceutical chemistry. The solid-state electron density, wich can be obtained experimentally by high-resolution X-ray diffraction, is a main source to gain these informations. During the last years, experimental charge density studies on 15 of the 20 natural amino acids have been performed and the results were compared with those obtained from various calculations [1].

Since the remaining ones are hard to crystallize in sufficient quality, we directed our interest to cocrystals with various solvents and we were able to measure high resolution X-raydata sets of L-phenylalanine and DL- and L-tryptophaneformic acid complexes [2],[3] which have the further interesting property to exhibit strong Speakman-type hydrogen bonds with D···A-distances <2.5Å.

The results of all so far known charge density studies of the natural amino acids are compared in terms of topological properties with special focus on the strong hydrogen bonds in the noted mixed complexes.

[1] Metta C.F., Bader R.F.W., *Proteins*, 2003, **52**, 360. [2] Görbitz C.H., Etter M.C., *Acta Cryst.*, 1992, **C48**, 1317. [3] Scheins S., Dittrich B., Messerschmidt M., Paulmann C., Luger P., *Acta Cryst.*, 2004, **B60**, 184.

Keywords: charge density studies, amino-acid complexes, hydrogen bonds