Comparative Charge Density Studies on Tripeptides of the Ala-Xxx-Ala-type

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A key concept in Bader's theory of 'Atoms In Molecules' (AIM) [1] is the transferability of topological electronic properties of submolecular fragments to macromolecular systems. In the biologically important class of amino acids and oligopeptides a considerable number of experimental charge density studies have been performed by high resolution X-ray diffraction. Transferability provided, these data can be used to derive electronic properties even for polypeptides or other polymeres, where crystals of sufficient diffraction quality can hardly be obtained.

The analysis of Ala-Xxx-Ala-type tripeptides is one of the steps following the path from small molecules to polymeric structures. Starting from Ala-Ala-Ala, the central amino acid was replaced by glycine, histidine and others. For that study, high resolution data sets ($\sin\theta/\lambda$=1.18Å) were collected in our group at 25K, respectively. The multipole refinements were accomplished with the program package XD [2]. The main attention was directed to the two different peptide bonds between Ala and Xxx in the zwitterionic molecules.

The transferability of the electronic properties could be extensively verified, but effects of the crystal packing are not negligible.

[1] Bader R.F.W., *Atoms in Molecules*, Clarendon Press, Oxford, 1994. [2] Koritsánszky T. et al., *XD*, *Freie Universität Berlin, User Manual*, 2001

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