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Crystal structures of hydrophobic dipeptides as hosts for organic solvent molecules

Carl Henrik Görbitz

Department of Chemistry, University of Oslo,Norway. E-mail: c.h.gorbitz@kjemi.uio.no

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The hydrogen bonding pattern in the crystal structure of a dipeptide is often dominated by two head-to-tail chains involving the N-terminal amino group and the C-terminal carboxlate group. The third amino H atom is then donated to a functional group in one of the side chains. If both residues have side chains devoid of such groups, as in dipeptides involving only Ala, Val, Ile, Leu and Phe (hydrophobic dipeptides), a strong tendency for cocrystalliization of hydrogen-bond-accepting solvent molecules is observed. Accordingly, crystal structures of hydrophobic dipeptides act as hosts for a range of organic solvent molecules (in addition to water). The peptide host framework includes various types of nanoporous structures [1-3] as well as structures divided into hydrophobic and hydrophilic layers [4,5]. New investigations focus on kiral recognition in these structures.

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Long Distances, Weak Interactions?

Mátyás Czugler[a]

[a]*Hungarian Academy of Sciences, Chemical Research Center, Hungary. 1525 Budapest, Hungary POB 17, E-mail: mcz@chemres.hu*

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Engineering crystals [1] and tailoring molecular properties [2], such as inclusion ability [3], molecular recognition [4], resolution by co-crystallization [5] and similar approaches require precise knowledge of governing interactions and other energetic and geometric properties [6] related to such experiments. One of these approaches involves systematic structural studies of weak interactions, such as the weak C-H ••• O hydrogen bridge types [7-9] or the rather weak C-H ••• (interactions [10]. These interactions are in some respects similar to either electrostatic interactions regarding vectorial properties or to van der Waals forces concerning their magnitude. Albeit subordinate in energy to strong intermolecular attractions, such as the classic hydrogen bridges [11] or ionic forces, these weak forces are usually more abundant and thus are also important. Although they have less directional nature and more dispersed character in space, it remains a challenge to describe the geometry and the absolute value of such *distance differences* between interacting moieties [9]. Recently, the crystal engineering approach makes extensive use of such analyses in a lot of analogous ways as reverse engineering does. A suggested [9] internal C-*H* ••• *O*=P hydrogen bridge was confirmed in a 1,2,3,6-tetrahydrophosphinine oxide derivative with exocyclic P=O bonds. Recently analysed salt-sugar complexes [12] also indicate balancing rôle of C-H ••• X type interactions.

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