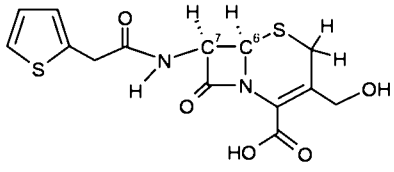
s9.m1.p3 **Hydrogen bond networks of solid cephalosporins - comparison with their biological activity.** I. Madura[1], J. Zachara[1], A. Zimniak[2], I. Oszczapowicz[3], [1]*Warsaw University of Technology, 00-664 Warsaw, Poland,* [2]*Medical University of Warsaw, 02-097 Warsaw, Poland,* [3]*Institute of Biotechnology and Antibiotics, 02-516 Warsaw, Poland*
Keywords: hydrogen bonds, absolute structure, cephalosporins.

Cephalothin, a widely used broad spectrum cephalosporin antibiotic[1], following parenteral administration to man and animals is converted in part to microbiologically less active metabolite, desacetylcephalothin[2]. In this work we present detailed analysis of the first crystallographicaly described structure of desacetylcephalotin: 7-[(2-thienacetyl)-amino]-3-desacetyl-cephalosporanic acid.

As most biologically active substances the compound is chiral and crystallises in monoclinic system in $P2_1$ space group symmetry. The absolute structure was established based on anomalous dispersion using the Flack parameter x.[3] The final x value of 0.05(9) confirmed well assumed model of the molecule of (6*R*, 7*R*) absolute configuration.



The tiophen ring was found to be disordered over two positions flipping along CH_2 C bond with s.o.f. 0.64 and 0.36. Analysis of molecular structure packing revealed strong intermolecular hydrogen bonds O H...O between the acid hydroxyl group and the peptide oxygen (O...O distance of 2.63(3) Å) and N H...O between the peptide imino and hydroxymethyl group (N...O 2.85(3) Å). Taking into account all important H-bonds the molecules are arranged in form of parallel helices oriented along the *b* axis.

The geometry of the main structure features is discussed and compared with parameters of previously described cephalotin sodium salt[4] and other cephalosporins structures found in Cambridge Structural Database. The main stress of the comparative study is put on close contacts and general attributes of the hydrogen bond network occurring in this metabolite and other cephalosporins and assigned to the biological activity.

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s9.m1.p4 **Formation of Highly Crystalline Guanidinium Salts of Sulfonated Phosphines and their Complexes.** A.Cs. Bényei,[a] Á. Kathó,[b] F. Joó,[b,c], [a]*Laboratory for X-ray Diffraction,* [b]*Institute of Physical Chemistry, University of Debrecen, and* [c]*Research Group on Homogeneous Catalysis, Hungarian Academy of Sciences, Debrecen 10, P.O.Box 7, H-4010 Hungary; e-mail: abenyei@delfin.klte.hu*
Keywords: guanidinium salts, hydrogen bond, templates.

Sulfonated triphenylphosphines, such as $Ph_2P(3\text{-}C_6H_4\text{-}SO_3Na)$, TPPMS and $P(3\text{-}C_6H_4\text{-}SO_3Na)_3$, TPPTS, are widely used in aqueous homogeneous and biphasic systems as ligands of transition metal containing catalysts. Organosulfonate anions form[1] crystalline salts with guanidinium ($guaH^+$) ion owing to the organised two-dimensional array of hydrogen bonds with participation of $-SO_3^-$ and $C(NH_2)_3^+$ units. We have prepared the guanidinium salt of TPPMS (TPPMS-guaH) *via* cation exchange in methanol and metal complexes. The two sulfonate groups in $[PdCl(TPPMS\text{-}guaH)]_2Cl_2$ point to the same direction favoured by the hydrogen bonding to $guaH^+$ ions and a layered structure is formed. Metathesis of TPPTS (Na-salt) with guaHCl also gave a crystalline compound but only two Na^+ were exchanged for $guaH^+$. Data acquisition routinely was performed at room temperature after packing single crystals into a drop of epoxy as freeze drying effect caused loss of solvate water molecules, hence decomposition of crystals even at 120K. Hydrogen bond networks in our compounds are compared with results of database search.

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