

Crystal Structure of a Polymorph of Carnidazole from Synchrotron X-ray Powder Diffraction

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The crystal structure of a polymorphic form of carnidazole, a nitroheterocyclic compound active against both anaerobic protozoa and bacteria, has been determined using synchrotron powder diffraction. The simulated annealing approach, as implemented in the program FOX [1], was used to obtain the initial model. The model was refined with the Rietveld refinement program Fullprof [2]. This monoclinic polymorph crystallizes in $P2_1/n$ space group with $a = 13.907(3)$, $b = 8.091(2)$, $c = 10.643(2)$, $\beta = 110.831(5)$, $Z = 4$. The imidazole ring is planar. The molecules are held in the crystal forming two infinite zig-zag chains along [010] via hydrogen bonds of the type N-H...N. A structural comparison with the previously reported polymorph and the monohydrate forms of this drug is presented.

[1] Favre-Nicolin V., Cerny R., *J. Appl. Cryst.*, 2002, **35**, 734. [2] Rodriguez-Carvajal J., 2001, *FullProf, version 1.9c*, LLB, CEA/Saclay, France.

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