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Monoclinic and tetragonal polymorphs of the sulfathiazole (1:1) adduct with pyridine

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In the two polymorphs of the sulfathiazole adduct with pyridine (1:1) (tetragonal, space group $P4_1$, and monoclinic, space group $P2_1/c$) the asymmetric units include sulfathiazole-pyridine dimers. The molecules of sulfathiazole are linked with each other via the $N_{aniline}H$ ... $O_{sulfato}$ hydrogen bonds to give infinite networks, different in the two adduct polymorphs (3D - in the tetragonal adduct, 2D - in the monoclinic adduct). N_{imine} is not participating in the formation of any hydrogen bonds in the structures of the adducts. In contrast to the structures of pure sulfathiazole, N_{amino} is not involved into formation of hydrogen bonds with other sulfathiazole molecules, being linked to pyridine, and as a result the frameworks formed by sulfathiazole molecules in the presence of pyridine guests is different from the networks formed in any of the five known polymorphs of pure sulfathiazole. Pyridine fills in cavities, being at the same time linked to the sulfathiazole network via hydrogen bonds $N_{amino}H$ ...$N_{pyridine}$. The adducts can be classified as inclusion compounds, with the host structures stabilized by the presence of the guest. Both polymorphs are not stable at ambient conditions and lose pyridine giving metastable polymorph I of sulfathiazole (m.p. 201.8 C, refcode suthaz01 in CSD). The single crystals of the tetragonal polymorph grow easily and reproduceably from n-propanol-pyridine solutions, whereas those of the monoclinic form were easily obtained for the first time, but could not be grown reproduceably later. The monoclinic form can serve as an example of the ”disappearing polymorphs”, thus suggesting that it is thermodynamically less stable, than the tetragonal adduct, although may grow easily due to kinetic reasons. The same polymorphs could be obtained by a solid + gas reaction of solid samples of sulfathiazole III (the stable modification at ambient conditions) with pyridine vapour. The process was monitored by powder X-ray diffraction in situ. At the first stage, a mixture of the adduct phases I and II was observed, which transformed on further exposure of the sample to pyridine vapour into adduct phase I (tetragonal).

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Further development of the general rule on correlation between host-guest ratio and topology of polymorphic inclusion compounds and their crystallization temperatures

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General rule correlating host-guest ratio and topology of polymorphic inclusion compounds with their crystallization temperatures has been formulated by us several years ago [1]: the high crystallization temperature of the polymorphic modification of the given host-guest complex the more close space occupied by guest molecules and the lesser an amount of the guest component. During past years many versatile host compounds were studied for this subject by our group and other investigators. These cases demonstrated correctness of the formulated rule. In the contribution the rule will be discussed involving these new examples and paying special attention to its practical significance.

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