by using the Pair Distribution Function analysis (PDF) together with structural Rietveld refinements to describe both the local structure and the long-range ordering.

[1] Martinetto, P. et *al.*, *J. Phys. Chem. B,* 110, 2006, 31, 15127-15133. [2] Pauchet, M. et *al.*, *Cryst. Growth and Design*, 4, **2004**, 6, 1143-1151. [3] Linol J. et *al.*, *Cryst. Growth and Design*, 7, **2007**, 9, 1608-1611.

Keywords: powder crystallography; organic pharmaceutical structure determination; pair distribution function

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Crystal Forms of Trospium Chloride. Michal Hušák[a], Michaela Hájková[a], Jan Čejka[a], Michal Dušek[b], Bohumil Kratochvíl[a]. [a]*Department of Solid State Chemistry, Institute of Chemical Technology, Prague, Czech Republic.* [b]*Institute of Physics, Academy of Sciences, Prague, Czech Republic.*
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Trospium chloride is a antispasmodic drug used to treat overactive bladder and symptoms of urinary incontinence, frequency, and urgency. The active substance is produced by crystallization from ethanol and declared as anhydrate. We tried to crystallize trospium chloride from several solvents with the main target – to determine the crystal structure used in production.
The structure of anhydrate was preliminary solved from synchrotron powder diffraction data (group $P2_1$, Z =2) by SA methods in DASH software and refined in Accelrys Reflex. Single crystals of anhydrite were obtained from ethanol. The structure of the single crystal at 150K has symmetry $P2_1/c$. Due to disorder the molecule is reflected by a pseudo-symmetry mirror plane x -y+1/2 z with the ratio between the two variants 4:1. The same disorder exists in powder data at room temperature but here the structure is non- centrosymmetric ($P2_1$), the c parameters is half and the ratio between the variants is approximately 1:1. The difference is probably caused by a phase transition (to be confirmed). The disordered structures were refined by Jana2006 using rigid body approach. The possibility of multiphase or twinned structure was tested and excluded
During the next crystallization experiments we had prepared single crystals of methanol and acetone solvates. Their structures were refined in $P2_1/c$, Z=4.
A comparison of all four known trospium chloride crystal forms is given.
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Keywords: trospium chloride; antispasmodic drug; solvates

FA4-MS09-P12

Hydrogen Bonding in Spirohydantoin Compounds. Shivachev Boris[a], Nikolova Rositsa[a]. [a]*Central Labolatory for Mineralogy and Crystallography, Bulgarian Academy of Science, Sofia, Bulgaria.*
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In order to fully explore structure activity relationships (SAR) around spirohydantoin scaffold, we have characterized structurally and biologically a variety of oxygen (O-1, O-2) and nitrogen N-3 substituents of the hydantoin moiety and varied the size of the cyckloalkane ring. We initially examined SAR around N-3 of the hydantoin core. We also attempted to improve the potency by thio substitution of carbonyl oxygen. The variation of SAR resulting from modification of the cycloalkane ring was also investigated. Incorporation of functional groups at N3, O1and O2 positions of the hydantoin ring resulted in complete turnaround of anti-convulsant activity. The SAR variation associated with cycloalkane ring modifications proved to be very flat, showing little improvement. As hydantoin ring structural parameters remain practically unchanged in all structures the SAR suggests that subtle changes in hydrogen bonding are responsible for the observed thorough changes of biological activity. This contribution will present a comparative study of hydrogen bonding patterns in the studied hydantoin compounds.

Keywords: hydrogen bonds in organic crystals; structure-activity relationships of drugs

FA4-MS09-P13

Pair Distribution Studies on Three Polymorphs of Paracetamol. C.A. Reiss[a], M. Gateshki[a]. [a]*PANalytical B.V., Lelyweg 1, 7602 EA Almelo, The Netherlands.*
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Recently the third polymorph of paracetamol was described [1]. Unit cell parameters and spacegroup were determined, but the crystal structure is not solved yet. It seems that some kind of disorder is present which makes it impossible to determine the structure up to now. In this study a different approach is taken to determine the structure of this third polymorph of paracetamol.
The total scattering pair distribution function (PDF) analysis is used to analyze structures on a local scale. This function looks at the absolute value of the distance between the nearest neighbours, the next nearest neighbours and so on. In the molecule of paracetamol the distances between the individual atoms are known giving the possibility to detect in the PDF of the polymorphs the differences of intermolecular interactions and disorder.
In this study the PDF's of the three polymorphs of paracetamol will be discussed and an attempted will be made to determine the structure of polymorph III.
The data is collected using a standard laboratory system with an X-ray tube with silver anode.

[1] C. A. Reiss and K. Goubitz, *Acta Cryst.*, **2008**. A64, C632

Keywords: polymorph; disorder; pair distribution function