

MS10-O3**Structural, spectroscopic and physicochemical investigations of new cocrystals of diamines and alcohols**Grzegorz Cichowicz¹, Łukasz Dobrzycki¹, Roland Boese², Michał Cyrański¹

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The aim of my study was to cocrystallize diamines, such as ethylenediamine and 2,2-dimethyl-1,3-propanediamine with various alcohols and determine structure of obtained systems. Both of the compound groups have enormous capabilities to form interesting structural motifs with many different substances. However in crystal structures of pure amines and alcohols there are often present chain motifs build by hydrogen bonds between amine or hydroxyl group [1]. Due to acceptor and donor properties both type of compounds are complementary and this fact can be promising in designing and obtaining new cocrystals of amines and alcohols with more complicated motifs and architectures. Using IR laser assisted in situ crystallization technique eleven new crystals was obtained [2]. Most of them crystallize in monoclinic system with 1:1 stoichiometry. All structures exhibit layered architectures consisting of pleated ribbons. The most primitive and repeatable motif in these arrangement is four-membered ring build by two amine and two hydroxyl group with a center of symmetry in the middle. However there are some structure with this motif but with other symmetry element, such us two-fold axis. The structure of pure of dimethyl-1,3-propanediamine has not been described due to formation of this amine the plastic phase in room temperature. Cooling down the sample causes phase transition between disordered F-centered cubic phase and I-centered tetragonal ordered phase. Similar situation is present in cocrystal of this amine with tert-butanol. In order to describe these phenomena's an hydrogen bond dynamics powder diffraction, differential scanning calorimetry and Raman studies were conducted.

References:

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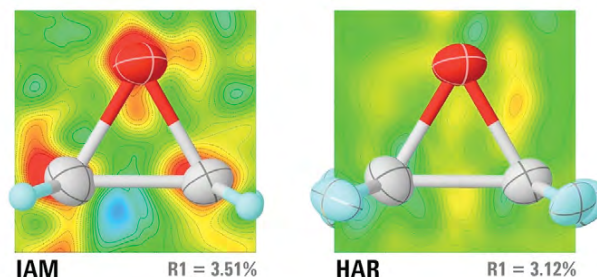
Keywords: diamines, alcohols, cocrystals

MS10-O4**Accurate hydrogen atom positions from standard X-ray Data: hirshfeld atom refinement and olex2**Horst Puschmann¹, Oleg Dolomanov¹

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“Hirshfeld atom refinement (HAR) is a novel X-ray structure refinement technique that employs aspherical atomic scattering factors obtained from stockholder partitioning of a theoretically determined tailor-made static electron density. HAR overcomes many of the known limitations of independent atom modelling (IAM), such as too short element–hydrogen distances, $r(X-H)$, or too large atomic displacement parameters (ADPs)” [1] HAR is now available in the general release version of Olex2 [2]. Given a standard X-ray dataset of good quality, information that could so far only be obtained by neutron diffraction can now be determined using HAR: accurate hydrogen atom positions. The residual electron density maps derived from this quantum crystallographic technique will also be much ‘cleaner’ than those obtained from standard Independent Atom Model (IAM) refinements. HAR is easy to run from Olex2, and in this contribution, I will introduce what HAR is, how it is implemented in Olex2 and how you run it. I will also discuss the current limitations of the technique. I invite you to try this at home: this presentation is available online and contains everything you need to know to get started [3]. Olex2 is open-source, available for Windows, MacOS and Linux and is free of charge.



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