

MS29-1-8 Crystallization and structural investigations of 1,2-cyclopentanediol analogues and their co-crystallization with ethylenediamine

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Abstract

Amine and hydroxyl groups, due to the complementarity of interactions, can form relatively strong hydrogen bonds, where the OH or NH₂ fragments can be both donor and acceptor [ref. 1]. Such interactions can be a driving force for the formation of a crystalline phase. However, the resulting structure can be affected by a presence of additional functional groups.

Presented here results are based on the crystal engineering of analogues of 1,2-cyclopentanediol and ethylenediamine. Since all the examined diols (*cis* and *trans* isomers of 1,2-cyclopentanediol and 1,4-anhydroerythritol) and their mixtures with ethylenediamine are liquids under normal conditions, the crystallizations experiments were performed *in situ* directly on the goniometer of the single crystal diffractometer with the use of an IR laser [ref. 2]. During the experiments a plastic and crystalline phase of *cis*-1,2-cyclopentanediol, a plastic phase of *trans*-1,2-cyclopentanediol and cocrystals of ethylenediamine with *cis*-1,2-cyclopentanediol and 1,4-anhydroerythritol were obtained and characterized by single crystal diffraction technique. For the neat diols DSC measurements were also performed. On their basis, the melting points of the compounds and temperature of the phase transition in the solid *cis*-1,2-cyclopentanediol were determined.

References

Ref. 1. O. Ermer and A. Eling, "Molecular recognition among alcohols and amines: supertetrahedral crystal architectures of linear diphenol–diamine complexes and aminophenols", *J. Chem. Soc. Perkin Trans. 2*, 1994, 925944.

Ref. 2. R. Boese, "Special issue on *In Situ* Crystallization", *Z. für Krist. - Cryst. Mater.*, 2014, 229, 595601.