Poster

The influence of reaction conditions on co-crystals of isoniazid derivatives

Mark G. Smith[1], **Andreas Lemmerer**[2]

1Department of Chemistry, University of South Africa, Florida, Johannesburg, South Africa;
2Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, South Africa

smithm2@unisa.ac.za

Co-crystals of covalently modified isoniazid were synthesized, using hydroxybenzoic acids as co-formers. During the co-crystallization of benzophenone derivatives of isoniazid, a small change in reaction or conditions played a large role in the outcome of the resulting supramolecular structure. The addition of either one or two methyl substituents to the benzophenone rings resulted in isostructural co-crystals. Changing the reflux time of the supramolecular synthesis resulted in stoichiometric variation. Adding larger quantities of one of the starting supramolecular reagents as “additives” resulted in polymorphism. Using an acid catalyst for the covalent modification of isoniazid during one-pot supramolecular synthesis prevented the formation of a solvate [1]. Supramolecular synthesis using mechanochemistry vs refluxing resulted in polymorphosm. Exposure to sunlight resulted in free radical polymerization of products [2]. In the presentation of this research paper [1], several unexpected results from changes in crystal conditions will be discussed.

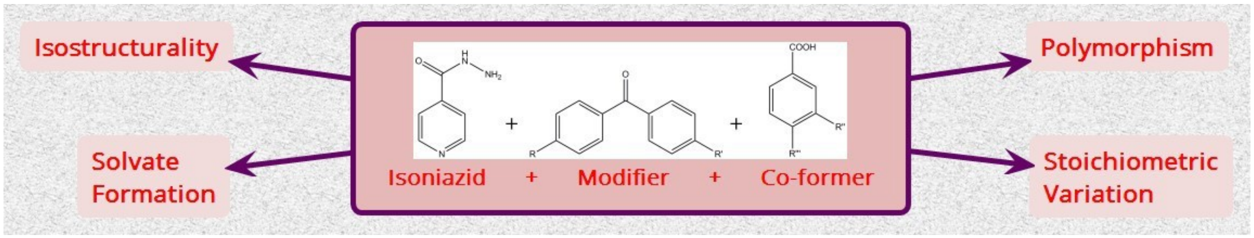

Figure 1. Change in reaction conditions resulted in stoichiometric variation [1].

[1] Smith, MG.; Lemmerer, A.; *Cryst. Growth Des.* (2018), **18**, 4777-4789.

[2] Smith, MG.; Lemmerer, A; *J.Mol. Struct*. (2019), **1179**, 132-144.