

Supramolecular synthon and conformational polymorphism in thiazole carboxamide compound

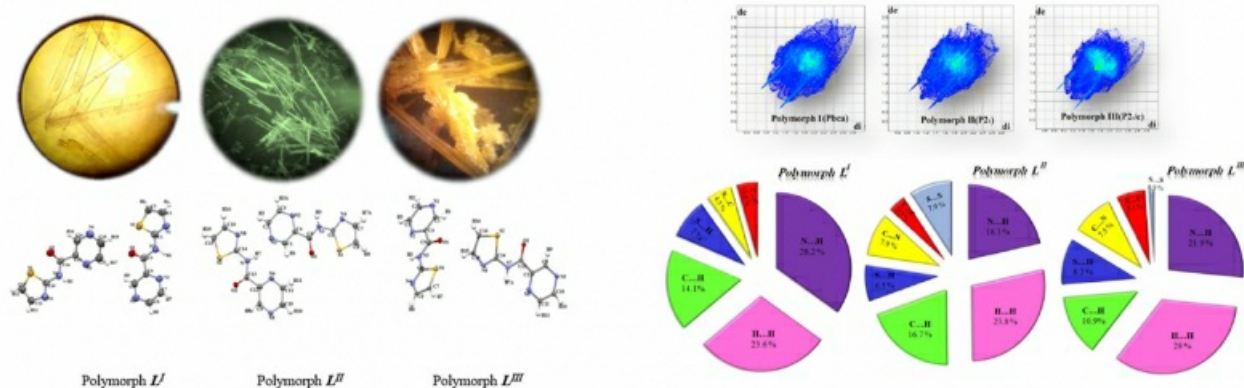
Fateme Tavakoli Ghouchani¹, Alireza Salimi¹, Behrouz Notash², Jered C. Garrison³¹Ferdowsi University Of Mashhad, Iran, Mashhad, Iran, Islamic Rep., ²Shahid Beheshti university of Tehran, Tehran, Iran, Islamic Rep., ³University of Nebraska Medical Center, USA, Nebraska, United States
E-mail: tavakoli.fateme@yahoo.com

Crystal engineering is based on the understanding of intermolecular interactions in a crystal packing and using of this understanding in design of new solids that involved in several subjects such as polymorphism. Polymorphism in crystals has been explained by McCrone as the ability of a substance to exist in at least two or more crystalline phases that they are different with each other in many aspects such as morphologies, melting point, IR spectroscopy, DSC analysis, and etc. In this study, design and synthesis of N-(1,3-thiazole-2-yl)-pyrazine-2-carboxamide compound (L) was accomplished and the product was initially characterized by CHNS microanalysis, IR, NMR and Mass spectroscopies and DSC analysis. While effort to obtain the suitable single crystal of titled compound, three polymorphic structures with variety of morphologies were discovered that the structures have been crystallographically determined by single crystal X-ray diffraction analysis (SCXRD). In the following, the crystal structures of polymorphs were investigated from crystal engineering viewpoint. The polymorphs are designed as polymorph LI, polymorph LII, polymorph LIII. The polymorph LI crystallizes in the orthorhombic space group, Pbc_a, whereas the polymorphs LII and LIII were crystallized in the monoclinic space groups P21 and P21/c, respectively. Investigations showed that the asymmetric unit of three polymorphs contains two independent molecules which have different orientations and interactions with each other. Flexible amide connection between pyrazine and thiazole rings results in the various conformations and different intermolecular interactions. So that the differences of structures arise from the orientation of the pyrazine and thiazole rings. The polymorphic structures have well arranged by donor and acceptor groups for effective supramolecular synthons. In order to indicate the percent and the important role of the interactions in LI-III crystal structures, Hirshfeld surface analysis, finger print plot and theoretical studies on dimer and tetramer moieties have been investigated. Exploring the stability energies related to the species being theoretically studied, emphasized to the role of hydrogen bonding interactions in the stability of polymorphic structures. It is interesting to notice that polymorphs LII and LIII contain very similar intermolecular interactions and the arrangement of synthons, whereas they have different orientations and crystal packing with each other. The results of theoretical studies confirmed the important role of hydrogen bonding and weak n-based interactions in the LI-III crystal structures.

[1] Desiraju, G. R. (2013) J. Am. Chem. Soc., 135, 9952-9967.

[2] Rahmani, M. et al. (2016) CrystEngComm, 18, 8953-8960.

[3] Phukan, N. et al. (2015). Crystal Growth & Design, 15, 1843-1851.

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