Solid state analysis and theoretical explorations on polymorphic and hydrate forms of *p*-hydroxybenzaldehyde isonicotinichydrazone: Effect of additives on polymorphic crystallization

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Abstract

The reaction of *p*-hydroxybenzaldehyde with an equimolar amount of isonicotinic hydrazide afforded two polymorphic and hydrate forms of *p*-hydroxybenzaldehyde isonicotinichydrazone (HBIH) by varying the experimental reaction conditions. The compounds are fully characterized by means of single crystal and powder diffraction methods, vibrational spectroscopy (FT-IR and Raman), thermal and elemental analysis. The compound crystallizes in three different forms in two different space groups, $P2_1/c$ (form P_A and P_B) and *P*bca (P_C). The Hirshfeld surface analysis shows the differences in the relative contributions of intermolecular interactions to the total Hirshfeld surface area for the HBIH molecules. The calculated pairwise interaction energies (104-116 kJ/mol) can be related to the stability of the crystals. Energy framework analysis identifies the interaction hierarchy and their topology. The geometry and conformation of the three forms are essentially similar which differ only by packing arrangement.

Keywords: *polymorphism, Raman spectroscopy, X-ray crystal structure, packing polymorphism, Hirshfeld surface analysis, energy frameworks*

1. Introduction

Polymorphism is the existence of a solid material in more than one form of crystal structure or phases that have different arrangements or conformations of the molecules in the crystal lattice. It offers a useful tool for examining the structure–property relationship due to the different intermolecular interactions and has received considerable attention from pharmaceutical industry and the academic community [1,2]. The difference in the internal structure of polymorphs alters their physicochemical properties, including

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