

Identification of a new polymorphic form of N-phenyl-2-(pyridin-4-ylcarbonyl)hydrazinecarboxamide: Structural insights by X-ray and quantum chemical calculations

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A new polymorph (**Form-II**) of N-phenyl-2-(pyridin-4-ylcarbonyl)hydrazine-carboxamide was synthesized and structurally characterized by single crystal X-ray diffraction analysis, and it was compared with another polymorphic form (**Form-I**). **Form-II** crystallizes in the orthorhombic system, space group $P2_12_12_1$ ($a=8.756(1)$ Å, $b=11.565(1)$ Å, $c=12.291(1)$ Å, $Z=4$ and $Z'=1$). The supramolecular networks of both polymorphic forms are stabilized by various intermolecular hydrogen bonding interactions, such as $N-H\cdots O$, $N-H\cdots N$, $C-H\cdots O$ and $C-H\cdots\pi$ interactions. In addition to these, $\pi-\pi$ stacking and lone pair (l.p) $\cdots\pi$ interactions contribute to stabilizing the solid-state structure of **Form-I**. A detailed analysis of Hirshfeld surfaces and 2D fingerprint plots was conducted to compare the intermolecular interactions. The lattice energy and interaction energies of both polymorphic forms were calculated using the PIXEL method. Furthermore, topological parameters derived from the 'atoms-in-molecules' (AIM) framework at bond critical points (BCPs) confirm the 'closed-shell' nature of non-covalent interactions. Additionally, a 'non-covalent interaction' (NCI) analysis was performed to identify intermolecular interactions.

Słowa kluczowe

Packing Polymorphism, Solid-state structure, Hirshfeld surface, PIXEL calculation, AIM's topology analysis, NCI analysis

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