

# High-pressure investigation of a cocrystal based on 4,4'-vinylenedipyridine and diphenic acid

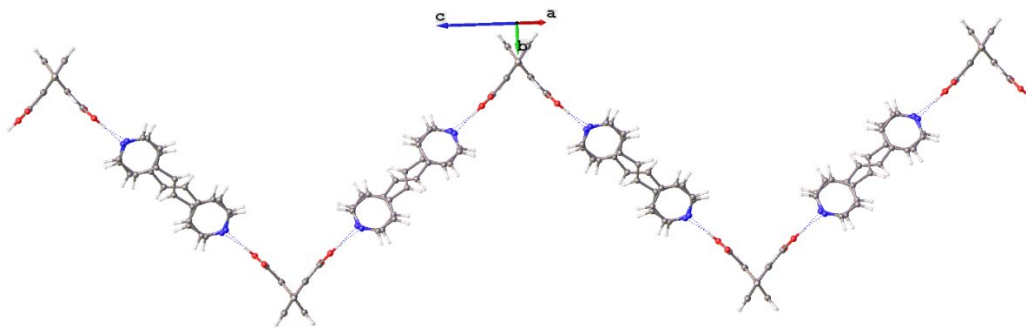
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Modification of the composition of the solid state by cocrystallisation allows to change physicochemical properties of solid state without the need for complex chemical reactions [1]. The selection of appropriate coformers is relatively straight-forward and is based on the analysis of the ability of the molecules of two different compounds to form compatible intermolecular interaction network [1]. However, the precise effect of cocrystallisation on solid form properties remains unpredictable [2]. In this context it is beneficial to investigate structurally-similar crystals which composition is only slightly modified to be able to locate and analyse key structural features behind differences in their properties. For instance, recent study of two isostructural cocrystals of 1,2-bis(4-pyridyl)ethane (ETY) with fumaric (FUM) and succinic (SUC) acids have revealed that seemingly insignificant change in number of  $\alpha$ -hydrogen atoms of acid molecules leads to major differences in the magnitude of negative linear compressibility (NLC) and phase stability [3,4]. In those cocrystals, NLC is associated with the deformation of a wine rack motif and reported study exemplifies how the exchange of the coformers allows for tuning of the NLC as long as the NLC-promoting motif remains undisturbed [4], an information useful for the design of organic NLC materials. Besides modification of the magnitude of NLC, crystal engineering approach can also be used to ensure formation of appropriate motif (e.g. wine rack, zig-zag), for example by employing compounds which molecules can change their conformation to mimic work of a hinge and at the same time can form H-bonds that direct molecular aggregation towards formation of NLC-promoting motif [5].

We present synthesis, crystal structure and high-pressure investigation of a new organic cocrystal based on 4,4'-vinylenedipyridine (VIN) and diphenic acid (DIP), where V-shaped molecules of DIP guide molecular aggregation towards formation of zig-zag chains (Fig. 1). The aim of the study was to assess how changes in the conformation of DIP affect deformation of the zig-zag motif and to compare the pressure response of VIN·DIP with that of structurally-similar cocrystal based on ETY and DIP. Analogous to previously reported cases of cocrystals of ETY with FUM and SUC, the difference between VIN·DIP and ETY·DIP lies in the hybridization of two carbon atoms forming a bridge between pyridine rings in VIN and ETY molecules, which affects their conformational flexibility.



**Figure 1.** Zig-zag motif formed by disordered VIN and DIP molecules in crystal structure of VIN·DIP at 0.1 MPa/298 K.

[1] Duggirala, N. K., Perry, M. L., Almarsson, Ö. & Zaworotko, M. J. (2015). *Chem. Commun.* 52, 640.

[2] Ding, Y., Zhao, Y. & Liu, Y. (2024). *Aggregate* e626.

[3] Patyk-Kaźmierczak, E. & Kaźmierczak, M. (2024). *Chem. Commun.* **60**, 10310.

[4] Patyk-Kaźmierczak, E., Szymańska, K. & Kaźmierczak, M. (2025). *IUCrJ* **12**, 88.

[5] Zeng, Q., Qiu, W., Li, C., Sun, Y., Hao, J. & Li, Y. (2024). *Phys. Chem. Chem. Phys.* 26, 15286.

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