

*Designing multi-component molecular crystals: A crystal engineering approach*

Mithun Paul<sup>1</sup>, Gautam R. Desiraju<sup>1</sup>

<sup>1</sup>Solid State And Structural Chemistry Unit (SSCU), Indian Institute Of Science., Bangalore, India

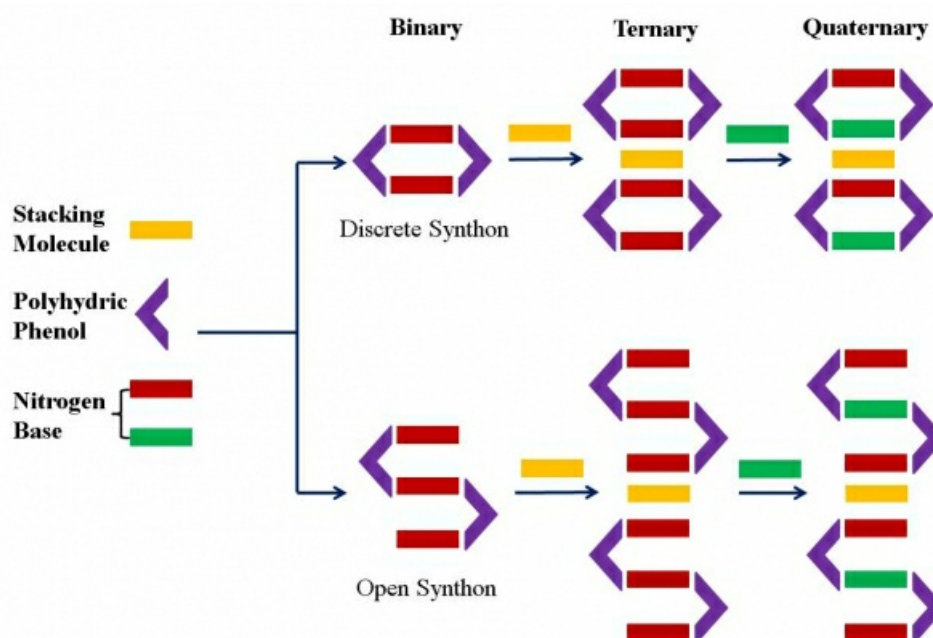
E-mail: ocmpiacs@gmail.com

Synthesis of multi-component molecular crystals or co-crystals has gained in importance in the field of crystal engineering because of their wide applications from materials to pharmaceutical sciences.<sup>1</sup> The past decade has witnessed an upsurge in this endeavor.<sup>2,3</sup> It is inherently difficult to introduce many components into the same crystal since crystallization of a mixture of compounds generally results in their separate crystallization. Despite this, several strategies have been implemented for the design of multi-component co-crystals based on robust supramolecular synthons. Here, a strategy is presented to obtain ternary and quaternary co-crystals of polyhydroxy aromatic compound with pyridine-like nitrogen bases and aromatic molecules that are prone to stacking. The moderately acidic phenolic proton easily forms co-crystals with nitrogen bases. The strong and robust phenol–pyridine (O–H•••N) synthon plays a major role in these systems to introduce modularity in the structures. After formation of the module, other weak interactions such as pi-pi stacking and C–H•••X (X = N/O) interactions contribute towards higher homologation of these co-crystals.

[1] Almarsson, O. & Zaworotko, M. J. (2004) Chem. Commun. 83, 1889-1896.

[2] Dubey, R. et al. (2016) IUCrJ 3, 102-107.

[3] Aakerøy, C. B. et al. (2011) Angew. Chem. Int. Ed. 40, 3240-3242.



**Keywords:** [Multi-component molecular crystal](#), [Supramolecular synthon](#), [Crystal engineering](#)