

# The Design and synthesis of ternary multi-component crystals through sublimation

**Matthew C. Scheepers, <sup>1</sup>Delia A. Haynes**

*Department of Chemistry & Polymer Science, Stellenbosch University, Matieland 7602, South Africa*

*mcscheepers@sun.ac.za*

Crystal engineering is the design and synthesis of new molecular solids with desirable properties and is an active area of research. Cocrystals are solid crystalline materials which contain two or more different neutral compounds coexisting in the same crystal structure. Many cocrystals are binary (i.e. consist of two coformers) but few are ternary (three coformers) or higher. Furthermore, most cocrystals are produced using solution-based methods (such as solvent evaporation), with very little work done on sublimation of cocrystals. Sublimation is the process in which a solid material transitions from the solid to gas phase (usually as a result of heating under vacuum), or the formation of solid directly from the gas phase (desublimation); usually in the cooler zone of a sublimation apparatus). This work explores the potential of the sublimation method to produce ternary multi-component crystals directly from the gas phase. We investigated the synthesis by sublimation of two ternary multi-component crystals that have been previously obtained using solution-based methods. The first multi-component crystal contains 3,5-dinitrobenzoic acid, 4-aminobenzoic acid and 4,4'-bipyridine [1] while the second contained 3,5-dinitrobenzoic acid, 3-aminobenzoic acid and isonicotinamide [2]. We also report a novel ternary multi-component crystal containing 3,5-dinitrobenzoic acid, 3-aminobenzoic acid and 4,4'-bipyridine, which was obtained from sublimation. Different experimental variables such as the sublimation temperature and stoichiometry were varied to determine which factors affect the formation of ternary cocrystals by sublimation.

[1] Seaton, C. C.; Blagden, N.; Munshi, T.; Scowen, I. J. (2013), *Chemistry A European J*, **19**, 10663–10671.

[2] Seaton, C. C., (2014), *CrystEngComm* **16**, 5878–5886