Array Crystallisation for Functionalised Organics using Different Variables

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We are currently exploring the crystallisation screening of functionalised organic compounds using an array reactor with solvent (x 4) and temperature (x 12) capability. Via this method we have prepared several crystals of 2,4-diamino-6-hydroxypyrimidine from water and methanol. Single crystal characterisation of the products has so far identified a pure form (monoclinic, $P2_1/c$, a = 7.688Å, b = 9.723Å, c = 7.419Å, β = 114.34°) plus two polymorphic mono hydrates (triclinic, *P-1*, a = 3.928Å, b = 8.660Å, c = 9.596Å, α = 83.23°, β = 88.15°, γ = 81.55°, and monoclinic, *C2/c*, a = 17.1571Å, b = 3.995Å, c = 18.682Å, β = 104.43°). The latter are both additional to one form previously described [1] on the Cambridge Structural Database (CSD) [2] (orthorhombic, Pbca, a = 16.721Å, b = 4.242Å, c = 18.293Å). Further work is in progress in this system and others; the results will be described in this poster.

[1] Skoweranda J., Bukowska-Strzyzewska M., Bartnik R., Strzyzewski W., *J. Crystallogr. Spectrosc. Res.,* 1990, **20**, (2), 117-121. [2] Allen F. H., *Acta Crystallogr. Sect. B,* 2002, **58,** 380-388.

Keywords: polymorphism, crystallisation, screening