

Crystallisation of oxcarbazepine form III : emergence of crystals with variable twisted habit.

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The emergence of crystal structures with twisted morphologies is well-documented [1]. Twisted single crystals have been observed nanoscopically, mesoscopically, and macroscopically and pose challenges with respect to structural characterisation as they lack long-range translational symmetry. Crystal structure prediction (CSP) capabilities can be employed in polymorph screening studies for aiding in the identification of thermodynamically feasible solid forms and assisting experimentalists in performing targeted screening [2,3]. Recent evidence suggests that combining CSP with powder X-ray diffraction data can assist in solving the structure of polymorphic crystals with twisted habit [4].

Keywords: oxcarbazepine; twisted crystal habit; crystal structure prediction

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