Influence of High Pressure on the Crystal Structure of Quinine Catalyst

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Crystal structures can undergo significant alterations when subjected to high pressure, including changes in molecular conformation, supramolecular assembly, and overall molecular organization [1]. In this study, the structural properties of a quinine-based organocatalyst and its solvatomorphs were investigated among other organocatalysts, under both ambient and high-pressure conditions [2–4]. Through detailed examination and comparison, valuable insights were obtained into the effects of high pressure on their crystal structures. The study revealed notable changes in key parameters, such as intermolecular interactions and packing arrangements, induced by pressure. While parameters such as unit cell volume, cell dimensions, and π–π interactions decreased under increasing pressure, an unexpected elongation of hydrogen-bonding distances was detected. Hirshfeld surface analysis further revealed a distinct trend: long-range interactions tend to shorten, whereas certain short-range interactions become elongated as pressure increases. These findings highlight the complex and non-linear nature of structural responses to high-pressure conditions. This work highlights the importance of pressure as a tool for tuning material properties and unlocking new functional possibilities.

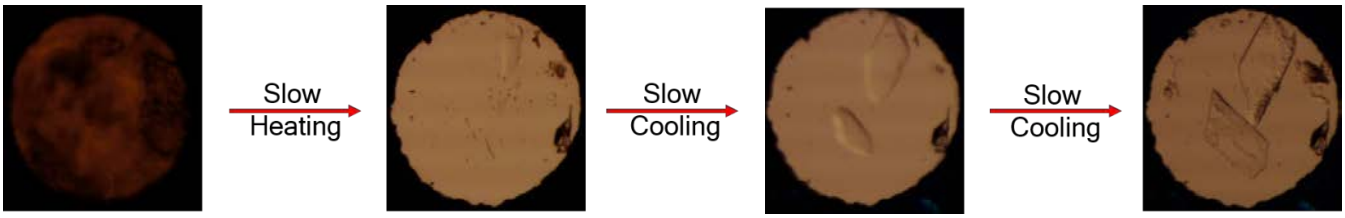

Figure 1. Crystallization of Quinine catalyst under high pressure (0.62 GPa) between room temp to 160°C temperature range.

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