Poster

Crystallisation of organic catalysts under different conditions and their main interaction patterns

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Research on organocatalysts has begun in recent decades, and their application in a growing number of new reaction pathways is expanding. Organocatalysts are not only being discovered for use in new areas but also offer a simplified operational scheme akin to enzymes. Crucially for industry, they provide an opportunity to move away from non-renewable heavy metals. Often, organocatalysts yield excellent results and can be used in various reactions with high efficiency and enantiopurity.

While the reaction products of organocatalysts are well-known and have been thoroughly analysed, and despite the extensive development of efficient catalysts and numerous theoretical calculations, the structural exploration of the organocatalysts themselves are limited. These interactions play a crucial role in crystal growth until we achieve a comprehensive understanding of typical interactions. In many cases, these interactions of appeared supramolecular interactions result in only one stable crystal conformation. However, by varying the substrates and environmental conditions, we can produce a variety of polymorphs of the reaction product, that continue to elucidate the characteristic interactions, thereby demonstrating their significance.

We investigated several organocatalysts (e.g.: thiourea and square acid amide based organocatalysts), and different crystal structures have been generated under varying conditions [1-3]. A few selected structures were also tested under high pressure. Once these crystal structures were obtained, their characteristic conformations and interactions were further explored.

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Tamas Holczbauer and Sourav De is grateful for the financial support from NEMZ_KI-00022 (National Research Development and Innovation Office).