Screening of Energetic Cocrystals using Thermal Analysis

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Cocrystallization is an important crystal engineering approach to design the diverse materials with improved functional properties. Cocrystal concept is well developed in pharmaceutical industry, but it is a relatively new for energetic materials design. In this study we compiled a dataset of previously published energetic cocrystals (ECCs), and categorized ECCs by the typical patterns of thermal behavior (ECC vs. neat coformers). Then for a smaller dataset (~30 entries) chemically diverse cocrystals we applied and modify the available thermal screening approaches. Finally, the unified procedure is reported, that meets the criteria of high-throughput screening. With the suggested approach the several pairs with promising energetic materials were screened and new cocrystals are found and reported.

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