MS29-1-2 Crystal engineering of phenol-phenolate supramolecular heterosynthon
#MS29-1-2

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Abstract
"Crystal engineering" is defined as "the field of chemistry that studies the design, properties and applications of crystals". One application of crystal engineering is prevalent in the study of cocrystals. Cocrystals have gained much attention, particularly in the pharmaceutical industry, due to their ability to modify physicochemical properties of drug molecules without changing their biological efficacy. Cocrystals are solids that are crystalline single-phase materials composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio which are neither solvates nor simple salts.[1] Cocrystals can be classified into molecular cocrystals (MCCs) that contain only neutral components (coformers) in the crystal lattice and ionic cocrystals (ICCs)[2] comprising of at least one ionic coformer that is a salt. ICCs involving inorganic salts (e.g., alkali and alkaline earth halides etc.) can also be viewed as a coordination complex between organic type ligands and metal cations. Ionic cocrystals have generated widespread interest as they exhibit strong hydrogen bonding or coordination bonding and have more components suggesting greater diversity of physicochemical properties.

The study of supramolecular synthons to investigate their amenability to crystal engineering will enable efficient discovery of new cocrystals. Supramolecular synthon is further classified into supramolecular homosynthon and heterosynthon.[3] Phenols are well-established in crystal engineering as they have demonstrated their ability to form robust supramolecular heterosynthons. They are also a common functionality found in many pharmaceutical and nutraceutical molecules. Phenol-phenolate ($PhOH\cdots PhO^-$) complexes have been studied in solution and gas phases but it remains understudied as a supramolecular heterosynthon in crystal engineering.

Statistical analysis on this $PhOH\cdots PhO^-$ supramolecular heterosynthon was conducted on relevant structures deposited on the Crystal Structural Database (CSD) and the novel ICCs reported in this work.

References
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