

Extending the structural space of quasiracemic materials

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Molecular shape is generally considered a prominent contributor to the formation of supramolecular assemblies. The role of this underappreciated structural feature to crystal packing, though, is often diminished or misconstrued in the presence of directional, more robust intermolecular forces. Quasiracemates – materials constructed from pairs of near enantiomers – offer important access to understanding molecular topology because the complementary shapes of the building blocks drive supramolecular formation. Our previous investigations in this area optimized quasiracemate formation by designing components with similar spatial properties. Here we report how systems with increased crystal lattice stabilization allow for greater topological differences of the quasiracemic components. The added stability in crystal packing is achieved by constructing molecular frameworks that are spatially larger (naphthylamides) or promote robust hydrogen-bonded assemblies (amino acids and carboxylamides). Data collected from these materials using X-ray crystallography, thermal analysis methods, and lattice energy calculations provide important insight into how these new molecular frameworks facilitate more significant structural variance of the component substituents during the pairwise assembly of quasienantiomers. Outcomes from this study also highlight a broader structure space towards the identification of new isostructural building blocks and essential topological relationships for quasiracemate crystallization.