

Departures from Near Inversion Symmetry Using Amino Acid Hydrogen Oxalate Quasiracemates

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Small-molecule quasiracemic materials have proven helpful for probing molecular shape-directed self-assembly. These materials consist of pairs of near enantiomers where the components often differ by slight chemical modifications (e.g., S-X/R-X'). When assembled, the pairs of quasienantiomers form motifs that mimic the inversion symmetry found in the related S-X/R-X or S-X'/R-X' racemic counterparts. Until recently, near centrosymmetric alignment held in spades for all known quasiracemic crystal structures. This study combines oxalic acid with several known amino acid quasiracemates to generate new ternary systems. Component cocrystallization of these materials results in robust supramolecular hydrogen oxalate chains with the amino acids attached to these motifs via strong N⁺-H···O and O-H···O contacts. While the core amino acid H₃N⁺-CH(C)-CO₂H fragments form near centrosymmetric alignment, several systems position the R groups without the anticipated close symmetry relationships. This diversion from inversion symmetry often relates to quasiracemates containing methionine, methyl cysteine, or ethyl cysteine. As part of the structure assessment process, both conformational similarity and degree of inversion symmetry of related pairs of quasienantiomeric components have been systematically studied to gain further insight into the molecular recognition process of these quasiracemic materials.