Microcrystal electron crystallographic analysis of organic solid solution (mixed crystal)

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Solid solution (mixed crystal) is a crystal containing a second constituent (with a variable ratio) which fits into and is distributed in the lattice of the host crystal (IUPAC). It is widely found among inorganic substances, but rarely among organic compounds because it generally forms an amorphous solid or, at best, tiny crystals with a low degree of crystalline order. We examined the potential of microcrystal electron crystallography for the study of a solid solution of a racemic mixture (pseudoracemate) of a new molecule that we synthesized recently. Diffraction data of rather poor quality were collected for numerous crystal-like particles, and optimized for various parameter including the R(F) value. The datasets collected from approximately 20 particles each containing R and S isomers in different ratios afforded the molecular structure as well as the crystal packing of the specimen of interest. In this lecture, we will also touch on our recent analysis of a supramolecular organic polymer that defied X-ray analysis. Reference: Bull. Chem. Soc. Jpn., 93, 776–782 (2020).