

Poster Presentation

MS67.P23

Structures and Properties of Diastereomeric Multi-component Crystals

D. Bock¹, C. Lehmann¹

¹*Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, Germany*

Multi-component crystals composed of two different chiral molecules have the potential to form diastereomers. In the present study a selection of chiral amides and acids was employed to form multi-component crystals. Since growing these multi-component crystals from solution failed, solvent assisted grinding was used. The resulting diastereomeric pairs, which are present as polycrystalline powders showed distinctly different powder diffraction patterns. In order to elucidate the crystal structures direct space global optimization structure solution methods were successfully used in several cases. A potential application of these diastereomeric multi-component crystals is the determination of the absolute configuration of one of the two components based on the known absolute configuration of the other.[1] In addition, Raman spectroscopy and DSC were employed to determine thermodynamic properties. In subsequent grinding experiments racemic conglomerates and racemates formed the starting material. These experiments demonstrated in several cases a relationship between melting point differences and preferential formation of only one diastereomer.

[1] D. A. Bock, C. W. Lehmann, *CrystEngComm*, 2012, 14, 1534-1537.

Keywords: chirality, ab-initio structure solution