

Mechanically Flexible Crystalline Diphenyl Urea Derives

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Controlling mechanical properties of crystalline organic materials remains a forbidden challenge despite their wide range practical applications.¹ We have recently demonstrated the importance of supramolecular shape synthons for designing mechanically flexible single crystals. We introduced active slip planes in crystal structures via different non-interfering supramolecular weak interactions (shape synthons), namely via van der Waals (vdW), p-stacking, and hydrogen bonding (OD) (carboxylic acid or amide) groups.² Here, we extend this design strategy to some diphenyl urea derivatives (as shown in figure 1), in which a linear one dimensional (1D) strong hydrogen-bonded chain is present while weak dispersive interactions (slip planes) are present in a perpendicular direction. 1D hydrogen bonded chains stack in the third dimension. The two N-H groups of one molecule form hydrogen bonds with the C=O of an adjacent molecule, while the vdW substituents such as methyl, chloro and bromo groups on either ends of the phenyl rings close pack to form slip planes. Mechanical behavior of the crystals was examined by a simple qualitative method, i.e. applying mechanical stress using a pair of forceps and a metal needle while viewing them under a stereomicroscope. Despite the presence of strong 1D hydrogen bonded network, the single crystals of 1 and 1a showed plastic flexibility on (0 0 2) and (1 0 0) respectively, while compound 2 underwent brittle fracture. This study highlights the utility of the vdW groups, which remained poorly explored in crystal engineering, for designing mechanically flexible dynamic single crystals.

References:

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