**Conglomerate Formation and Crystal Structure of 1,3-Oxazolidin-2-one Derivatives.**

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Homochiral 1,3-oxazolidin-2-ones and their thioxo analogs have been used as versatile and efficient chiral auxiliaries in asymmetric synthesis. (Fig. 1) We have focused our research interest on their optical resolution through preferential crystallization. This methodology is dictated by the formation of conglomerate crystals from the racemate solution. Factors that lead to the formation of a conglomerate are poorly understood and the crystallization condition is examined in the trial-and-error approach. Knowledge of crystal structures of chiral and racemic species is important for the design of the conglomerate crystallization. In searching for the crystallization condition, we have found that racemic 4-phenyl-1,3-thiazolidin-2-one (4-PTO) crystallizes as conglomerates. In this work, we have analyzed X-ray crystal structure of 4-PTO in order to understand the structural factors leading to the conglomerate formation. The structural features are also compared with those of 4-POO, 4-POT and 4-PTT reported previously [1].

Fig. 2 shows the crystal structure of conglomerate 4-PTO. The N-H…O intermolecular hydrogen bonds are formed between the amide groups of neighboring molecules, which results in a homochiral infinite zigzag chain structure around 2-fold screw axis along the b. In addition, intermolecular S…O close contacts are observed between the thioether sulfur atoms and the carbonyl oxygen atoms in this chain structural unit. Homochiral PTO molecules are closely packed each other through these intermolecular interactions. Moreover, T-shaped stacking interactions are observed between the homochiral chains. Thus, the crystal structure of conglomerate 4-PTO can be regarded as a homochiral supramolecular assembly of infinite chain structural units.