Hydrogen bonding networks of chiral diacids and their derivatives

W. Chant and D.R. Turner

School of Chemistry, Monash University, Clayton, VIC 3800, Australia
wcha0069@student.monash.edu

Keywords: hydrogen bonding, chirality, crystal engineering

Chiral materials have potential applications as solid phases in enantioselective separations, or as parts of hydrogen-bonding salt components for enantioslective crystallisation. One major pitfall is that the ligands used must themselves be enantiopure and, ideally, not cost-prohibitive to synthesize. Our approach has been to use naphthalenediimides (NDIs) and related, shorter diimide species, that are appended by amino acids at the imide positions, thus being accessible as an enantiopure product in a one-step reaction from a dianhydride precursor.

We have found that chiral ligands containing this NDI core (Figure 1, left) reliably form a metallomacrocyclic motif as part of coordination polymers [1]. Furthermore, the window within these macrocycles is the ideal size to accommodate an aromatic guest, including catenation with other macrocycles and formation of rotaxanes using linear co-ligands (Figure 1, right). We have successfully translated these motifs from the solid-state into solution [2], and demonstrated the reliance of supramolecular motifs on the nature of the ‘R’ group of the amino acid [3]. As such, they have proven useful from a crystal engineering perspective. The use of different core groups, either smaller, more flexible or bent, lead to radically different materials, typically discrete complexes including lantern-type cages and polyhedral [4].

Here, we report a series of hydrogen bonding networks of both the neutral chiral diacids and salts containing their dicarboxylate derivatives.

Figure 1. (Left) Naphthalenediimides appended with amino acids reproducibly form macrocyclic motifs within coordination polymers, due to conformational preferences of the ligand, which are conducive to crystal engineering of interlocked networks. (Right) A framework containing a shorter, chiral diimide ligand has been shown to selectively host one enantiomer of 1-phenylethanol using crystallography.