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Controlling size and chirality of supramolecular cage complexes

A series of chiral coordination cage complexes has been synthesised using amino acid substituted diimide ligands. Using a biphenylsulfonediimide core (BPSD) substituted with amino acids, a series of quadruple stranded Cu4L4 cages have been formed. The cages contain two copper paddlewheel units connected by four ligands. Analogous chiral complexes (helicates) and achiral complexes (mesocates) can be formed by controlling or removing the stereocentres within the ligands(1). Enantiopure leucine-substituted ligands (LeuBPSD) form helicates, complexes which have supramolecular chirality due to a twist in the ligands. Swapping the handedness of the amino acid ligand forms the opposite handedness helicate cage complex. The helicate cages are self-selecting, as the reaction of the (R,R) and (S,S) ligands with Cu(II) forms a mixture of enantiopure cages, with no product containing both ligands. Removing the chirality of the ligand, by using a BPSD ligand substituted with achiral amino acid, glycine (GlyBPSD), or using the (S,R)-LeuBPSD ligand, leads to the formation of mesocates, which lack supramolecular chirality. The cage complexes formed with BPSD ligands have an internal void volume of ~300 Å3. The use of alternative diimide amino acid substituted ligands have also been shown to form larger and more complex chiral supramolecular cages, which have an internal void volume of up to 1000 Å3, establishing the possibility of chiral catalysis and separation applications for these complexes.

Keywords or phrases (comma separated)

Chiral, supramolecular, cage, helicate, crystallography

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