



Hierarchical Self-Assembly of Supramolecular Helical Fibres from Amphiphilic C₃-Symmetrical Functional Tris(tetrathiafulvalenes)

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Résumé en anglais

The preparation and self-assembly of the enantiomers of a series of C₃-symmetric compounds incorporating three tetrathiafulvalene (TTF) residues is reported. The chiral citronellyl and dihydrocitronellyl alkyl chains lead to helical one dimensional stacks in solution. Molecular mechanics and dynamics simulations combined with experimental and theoretical circular dichroism support the observed helicity in solution. These stacks self-assemble to give fibres that have morphologies that depend on the nature of the chiral alkyl group and the medium in which the compounds aggregate. An inversion of macroscopic helical morphology of the citronellyl compound is observed when compared to analogous 2-methylbutyl chains, which is presumably a result of the stereogenic centre being further away from the core of the molecule. This composition still allows both morphologies to be observed, whereas an achiral compound shows no helicity. The morphology of the fibres also depends on the flexibility at the chain ends of the amphiphilic components, as there is not such an apparently persistent helical morphology for the dihydrocitronellyl derivative as for that prepared from citronellyl chains.

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