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Neutral interlocked assemblies from anionic pseudorotaxanes coordinated to Sn(IV) and Cu(I) metallic centers

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Abstract

Anionic [2]pseudorotaxanes have been prepared by threading an axle consisting of two dithiophosphate donor groups attached to a 1,4,5,8-naphthalenediimide (NDI) core through the cavity of the bis-1,5-(dinaphtho)-38-crown-10 ether (15DN38C10). The subsequent coordination of these interlocked, negatively charged species to R_3SnCl ($R = Me, Ph$) and $(Ph_3P)_2CuNO_3$ yields neutral (pseudo)rotaxanes of the general formula $NDI[(CH_2CH_2O)_n(An)PS_2^-\text{"M"}]_2 \subset 15DN38C10$ ($n = 1, 2$; $An = anisole$; $\text{"M"} = R_3Sn \text{ or } (Ph_3P)_2Cu$). Solution and solid state studies of the rotaxation process show that there are two factors influencing the interaction between the axles and the wheel: the *size* of the stopper and the *length* of the side-arms of the axles. When the axle termini are bulky enough to prevent threading, the length of the side-arms has little influence over the self-assembly process. In contrast, when the size of the stopper does not preclude the threading of the axle through the cavity of the crown, the length of the side-arms is the determining factor in the rotaxation process. These results presented here provide an alternative method for the synthesis of counter-ion free interlocked species, based on *anionic axles* with donor capabilities that would produce a neutral interlocked architecture upon threading and coordination to *cationic metal-containing centers*.

Keywords:

Pseudorotaxanes; Supramolecular chemistry; X-ray crystal structures; Phosphor-1,1-dithiolates; Metal complexes.

Highlights:

- Anionic pseudorotaxanes have been prepared.
- Their propensity to coordinate to Sn(IV) and Cu(I) centers has been explored.
- Neutral bimetallic interlocked architectures have been obtained.
- Solution and solid state (X-Ray diffraction) studies were performed.

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