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News Item

Picking Up the Chemical Thread

Threading the molecular needle – passing a linear molecule through a cyclic one – is an old trick: 'hooplane', an alicyclic ketol on a hydrocarbon axle, was fashioned in 1967 by researchers at Syntex Research in Palo Alto, and the term 'rotaxane' for these rotor-and-axle assemblies dates back to Gottfried Schill's similar construction in 1980. But whereas these were the products of conventional ring-closure syntheses, the principles of supramolecular host-guest chemistry are now making the molecular gymnastics of rotaxane synthesis far easier. The extent to which this is true should be apparent from the supramolecular complex (Fig. 1) described by A. Harada *et al.* [*Nature* **356**, 325 (1992)] which contains twenty or more cyclodextrin rotors on a strand of polyethylene glycol.

A wide variety of threaded supermolecules has been developed in recent years, many by Fraser Stoddart's group and Jean-Pierre Sauvage and colleagues. Stoddart has used linear and cyclic paraquat–hydroquinone complexes to create the 'molecular shuttle', a rotaxane in which the rotor can switch between two docking points on the thread, and a range of catenanes, in which the ends of the thread are joined. A single bead threaded on a long loop with several docking points constitutes a 'molecular train' that can circle around the line until cooled to a standstill. Stoddart

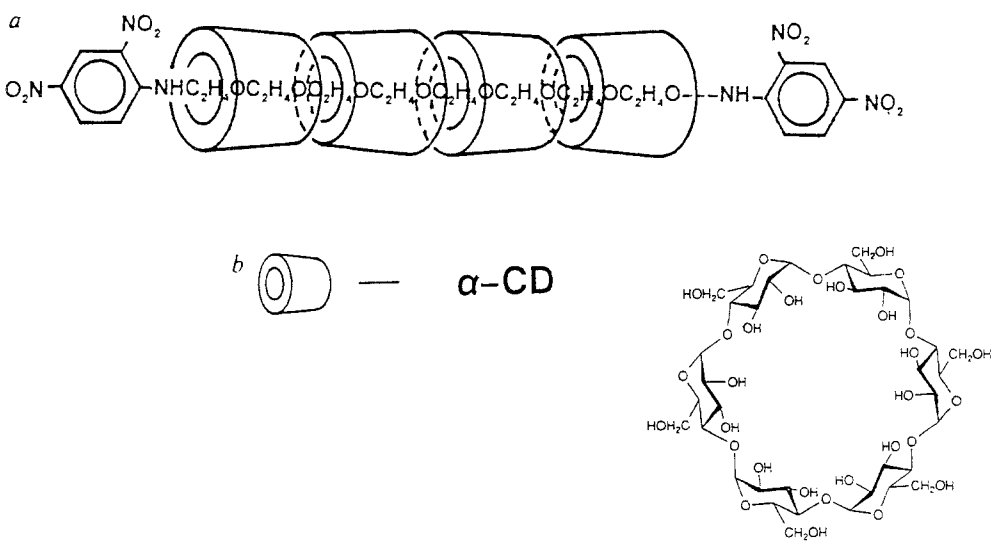

Fig. 1. (a) Molecular necklace prepared from complexes of poly(ethylene glycol) bisamine with α-cyclodextrins by capping the complexes with 2,4-dinitrofluorobenzene. (b) α-Cyclodextrin.

has made the whimsical suggestion that several beads on a strand might constitute a 'molecular abacus'.

The complex synthesized by Harada *et al.* shows that this is easier than might be supposed. The components are simply mixed in aqueous solution, and the resulting complex is capped at each end with 2,4-dinitrofluorobenzene. Diffraction and spectroscopic studies of the crystalline form confirm that it is a 'molecular necklace'. The polymer thread is about 266 Å long, and the cyclodextrins occupy only about 160 Å or so of this length – Harada *et al.* suspect that each sticks closely to its neighbours via hydrogen bonding when in the solid state, but that the molecular beads are mobile when the complex is in solution. P.B.