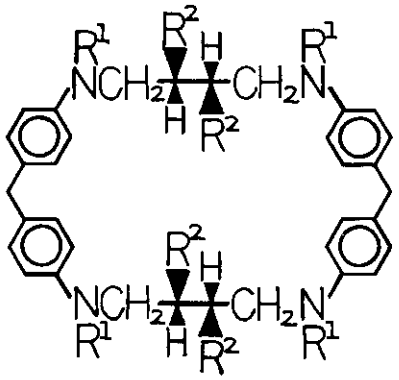
HOST-GUEST COMPLEX FORMATION BY AN OPTICALLY ACTIVE PARACYCLOPHANE IN WATER

Ichiro Takahashi, Kazunori Odashima, and Kenji Koga*

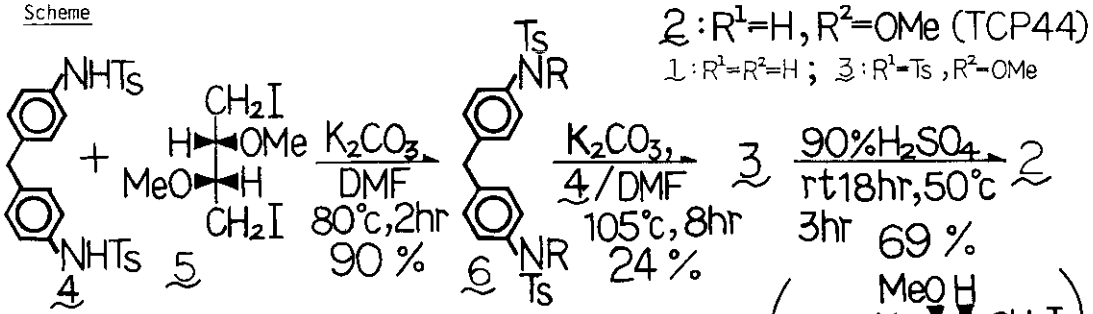
Faculty of Pharmaceutical Sciences, University of Tokyo

Hongo, Bunkyo-ku, Tokyo 113, JAPAN

Previously we have reported the crystallographic[1] and NMR spectral[2] studies showing that CP44 (1), soluble in acidic water (pH<2), forms inclusion host-guest complexes with hydrophobic "aromatic" guests in a particular geometry. For application of this system to asymmetric reactions, we carried out the synthesis of TCP44 (2), containing the units derived from L-(+)-tartaric acid (Scheme): This is the first synthesis of a chiral, water-soluble paracyclophane.



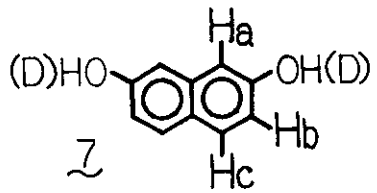
Scheme



In DCl-D_2O (pD 1.2) host 2, as well as host 1, induced marked upfield shift on ^{1}H NMR signals of guest 7, showing that host 2 forms a strong complex, comparable to that by host 1 (Table). Under similar conditions, formation of diastereomeric complexes between 2 and D-/L-mandelic acid is evidently observed. Further studies aiming asymmetric synthetic reactions are now in progress.

Table Changes of ^{1}H NMR chemical shifts of 7

Host	Δδ(Ha)	Δδ(Hb)	Δδ(Hc)
2 (pD 1.2)	−1.75	−0.61	−1.62
1 (pD 1.2)	−1.90	−0.59	−1.75



$\Delta\delta_{ppm}$ = δ(Host+Guest)−δ(Guest), [2]=[1]=5.0x10^{-2}M, [7]=2.5x10^{-2}M, in DCl-D_2O (pD 1.2).

1) K. Odashima, A. Itai, Y. Iitaka, and K. Koga, J. Am. Chem. Soc., 102, 2504 (1980).

2) K. Odashima, A. Itai, Y. Iitaka, Y. Arata, and K. Koga, Tetrahedron Lett., 21, 4347 (1980).