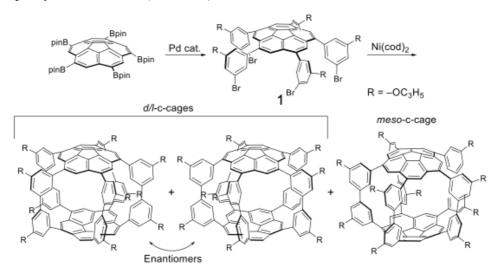
Development of Corannulene-based Covalent Cages

(Graduate School of Science and Technology, Nara Institute of Science and Technology) OHaruka Kano, Hiroko Yamada, Naoki Aratani

Keywords: Corannulene, Caged compound, Chirality

Synthetic covalent cages having a well-defined inside cavity have received great interest, since those molecules can stably encapsulate guest molecules inside and are more rigid than supramolecules. In this study, we succeeded in the synthesis of five-fold biphenylene-bridged corannulene dimers (c-cages) by the nickel-mediated homo-coupling of a pentakisbromophenyl corannulene 1 (Scheme 1).



Scheme 1. Synthesis of d/l and meso-c-cages.

The products were mixture of d/l and meso **c-cages**, and their separation was achieved by HPLC. Each c-cage incorporates a single molecule of DMF used as co-solvent which was confirmed by ¹H NMR and single-crystal X-ray analysis (Figure 1). The enantiomers of the d/l c-cage were optically separated by chiral HPLC, which gave the mirror-image circular

dichroism (CD) spectra. Encapsulation of other guest molecules was investigated to check the guest-dependent physical properties of c-cages.

Figure 1. Single crystal X-ray structures of a) *d/l* and b) *meso* **c-cages**.