

Development of Novel Heterocyclic Compounds and Their Molecular Assemblies for Advanced Materials

Safety Office



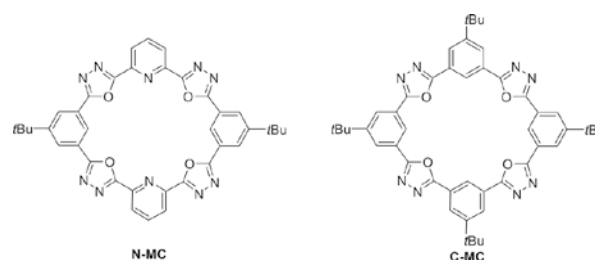
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Heterocycles containing sulfur and/or nitrogen atoms are useful as components of functional organic materials since heteroatoms in their rings are helpful to stabilize ions or ion-radical species. In addition, intermolecular interactions caused by heteroatom contacts can be expected to form unique molecular assemblies. In this project, novel functional organic materials based on various heterocycles were synthesized and their physical and structural properties were investigated.

1. Synthesis and Crystal Structure of a Novel Macrocyclic Compound for a Supramolecular Nanotube¹⁾

The novel macrocyclic compound (N-MC) was synthesized as a nitrogen analog of a macrocyclic compound (C-MC).

The crystal structure of N-MC was investigated by an X-ray crystallographic analysis, and the crystal was characterized by a step-like columnar structure, which is different from the supramolecular nanotube structure of C-MC. The molecular framework and the number of *tert*-butyl groups affected the molecular arrangement in the crystal.



Reference

- 1) K. Ono, S. Karasuda and M. Tomura, *Heterocycles* **94**, 2209–2214 (2017).

Multifunction Integrated Macromolecules for Molecular-Scale Electronics

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Recently a single electron tunnel device (SET) has attracted much attention as an ultra-low-power device. In this project, to establish an innovative fabrication process for SET systems, we have been developing step-wise synthetic protocols for mono-molecular single-electron tunnel devices and their integrated circuits (MOSET IC).

1. Efficient Step-Wise Chain Extension of Rigid-Rod Linkers for Molecular Framework

We have developed an efficient synthetic route for step-wise chain extension of rigid-rod linkers (1-4). Figure 1 illustrates the synthetic scheme. In Sonogashira reactions, the removal of diacetylene by-product is frequently time consuming, but in our scheme, the separation is easy based on the difference in polarity of the silyl protecting groups.

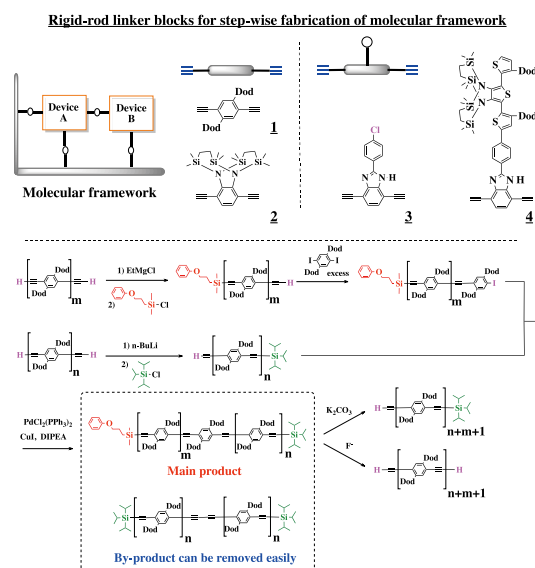


Figure 1. Representative synthetic scheme for step-wise chain extension of building blocks 1-4.