2023 CSJ Annual Application form

Category

大分類：12 Organic Chemistry -Organic Crystals, Supramolecular Chemistry-
中分類：Oral A
小分類：self-assembly and molecular recognition
発表言語：English

Keywords (four)
molecular self-assembly, cage complexes, self-assembly process, palladium

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Title

Kinetic template effect on the self-assembly process of Pd_2L_4 cage consisting of ditopic pyridyl ligands with a 1,3-phenylene spacer

Synopsis（not more than 100 words）

The self-assembly process of the Pd_2L_4 cage from Pd(II) ions and ditopic pyridyl ligands with a 1,3-phenylene spacer (L) was investigated by QASAP. It was found that appropriate template anions (NO_3^- or BF_4^-) are required for the self-assembly to reduce the electrostatic repulsion between the two Pd(II) ions in the cage. Long-lived intermediates were also observed by ^1H NMR spectroscopy during the self-assembly. Some of these species, such as $Pd_2L_2X_4$ ring and $Pd_2L_3X_2$ partial cage (X: leaving ligand), were separately prepared under kinetic control and were used for detailed analysis of the self-assembly mechanism.

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