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Single crystal x-ray structures of coordination-driven self-assemblies

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In recent years, coordination-driven self-assembly has become a dominant method for constructing 2D and 3D supramolecular architectures. These supramolecular architectures are fascinating not only because of their structural beauty and topological importance but also because of their application in catalysis, host-guest chemistry, molecule recognition, and drug-delivery. Our group has reported a number of complex supramolecular topologies such as [2] catenane or Hopf link, Solomon links, Borromean rings, ring-in-ring and very recently a molecular knot 818 using this method. Due to the structural complexity, determination of structure by conventional spectroscopic techniques is not possible, therefore, single-crystal X-ray analysis remains the only technique to establish the structure. Suitable single crystals for X-ray diffraction analysis were obtained by the vapor-diffusion method. Coordination-driven self-assembly of tetracene-based Ru(II)-acceptor and 1,4-bis(4-pyridylethynyl)tetrafluorobenzene donor along with the non-covalent interactions ($\text{CH}\cdots\pi$ and $\pi-\pi$) results in the formation of a molecular Borromean ring, as revealed by synchrotron X-ray diffraction analysis (Fig 1). After establishing the solid-state structure, other complimentary spectroscopic techniques such as ^1H NMR, ^{13}C NMR, and ^1H DOSY, along with ESI-MS and elemental analysis were used to fully establish the structure in solid as well in solution state.

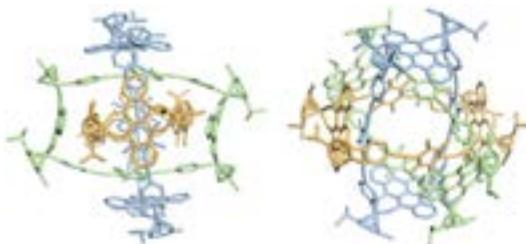


Fig1. Crystal structure of coordination-driven self-assembly of 1,4-bis(4-pyridylethynyl)tetrafluorobenzene donor with an arene ruthenium acceptor.

Biography

Dong Hwan Kim was born in Ulsan, Republic of Korea in 1989. He obtained his master's degree in chemistry from the University of Ulsan in 2016 and thereafter he started his PhD studies at the same University under the guidance of Prof. Ki-Whan Chi. His research interest is in the area of molecular topology via coordination-driven self-assembly.

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