Structural Determination of Polycyclic Ether via Conformational Fixing in a Cage

(*[1]Graduate School of Engineering, The University of Tokyo*, *[2]Division of Advanced Molecular Science, Institute for Molecular Science, [3]UTIAS, The University of Tokyo)*
○Yikuan Yu,[1] Wei He,[1] Kenta Iizuka,[1] Hiroki Takezawa,[1] Makoto Fujita[2,3]

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The structural study of five-membered rings is of great significance, as these structures are commonly found in key compounds of chemical and biological research. However, five-membered rings possess many conformations, making it nearly impossible to reliably depict these structures. In this work, we employed two coordination cages to encapsulate polycyclic ethers with five-membered rings to form host-guest complexes for crystallographic studies. The host-guest interaction leads to the stabilization of specific conformations of the five-membered rings, allowing for the clear structural determination of highly flexible molecules containing multiple five-membered rings.

An octahedral M_6L_4 cage was utilized to encapsulate the cyclic diether series and was crystallized by adding organic polysulfonates as crystallizing agents. The stereostructures were obtained through single crystal X-ray diffraction. Compared with the structural results based on the crystalline sponge method, in which guest molecules pack loosely, the M_6L_4 cage showed an improved electron density of guest molecules, which could be due to the conformational fixing inside the cage. An enlarged M_9L_6 cage was used to encapsulate polycyclic ether salinomycin, and conformational fixing on this natural polycyclic ether compound shows the potential of absolute structural determination of large, flexible molecules using the M_9L_6 cage.

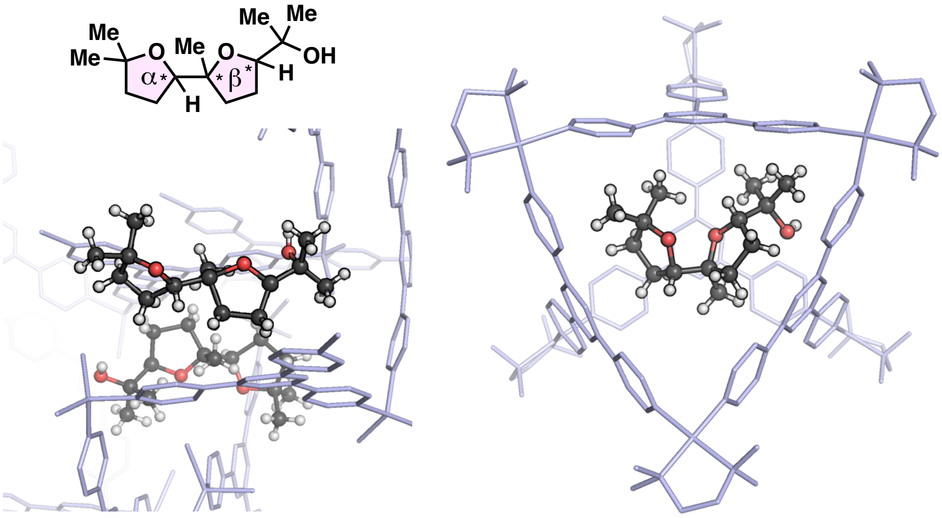

Fig. 1. Crystal structures of a cyclic diether measured through encapsulation in a crystalline sponge and M_6L_4 cage.