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NOVEL MACROCYCLES WITHIN MACROCYCLES: CYCLEN, CYCLAM AND THEIR TRANSITION METAL COMPLEXES ENCAPSULATED IN CUCURBIT[8]URIL

*Soo-Young Kim and Kimoon Kim**

National Creative Research Initiative Center for Smart Supramolecules and Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, San 31 Hyojadong, Pohang 790-784, Republic of Korea

Our recent discovery of new cucurbituril homologues, cucurbit[n]uril (CB[n]; n = 5, 7, and 8), containing five, seven, and eight glycoluril units has opened up new opportunities to expand the host - guest chemistry of cucurbituril. The largest member of the cucurbituril family, CB[8], has a cavity comparable to that of -cyclodextrin and can accommodate two aromatic guest molecules to form 1:2 host - guest complexes, or 1:1:1 ternary complexes.

And CB[8] also forms 1:1 host-guest complexes with protonated cyclen (1,4,7,10-tetraazacyclododecane) and cyclam (1,4,8,11-tetraazacyclotetradecane). The X-ray crystal structures of the complexes (1 and 2, respectively) confirms that a protonated macrocycle resides in CB[8] reminiscent of Russian *Matrioshka* dolls. The macrocycles inside CB[8] in 1 and 2 can be metalated with transition metal ions. The X-ray structures of the Cu complexes (3 and 4) reveal that Cu(II)(macrocycle)(H_2O) resides inside the cavity of CB[8]. The complex 3 contains a five-coordinate Cu(II) in a square-pyramidal environment, with the Cu ion being 0.66 Å above the average plane of the four N atoms of cyclen. An electrochemical study shows the encapsulation of Cu(cyclen) in CB[8] increases stability of the Cu(I) state but considerably slows down the electron transfer between electrode and the redox center.