**Poster Presentation**

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## *Guest Inclusion Crystal structures of Macrocyclic Boronic Esters*

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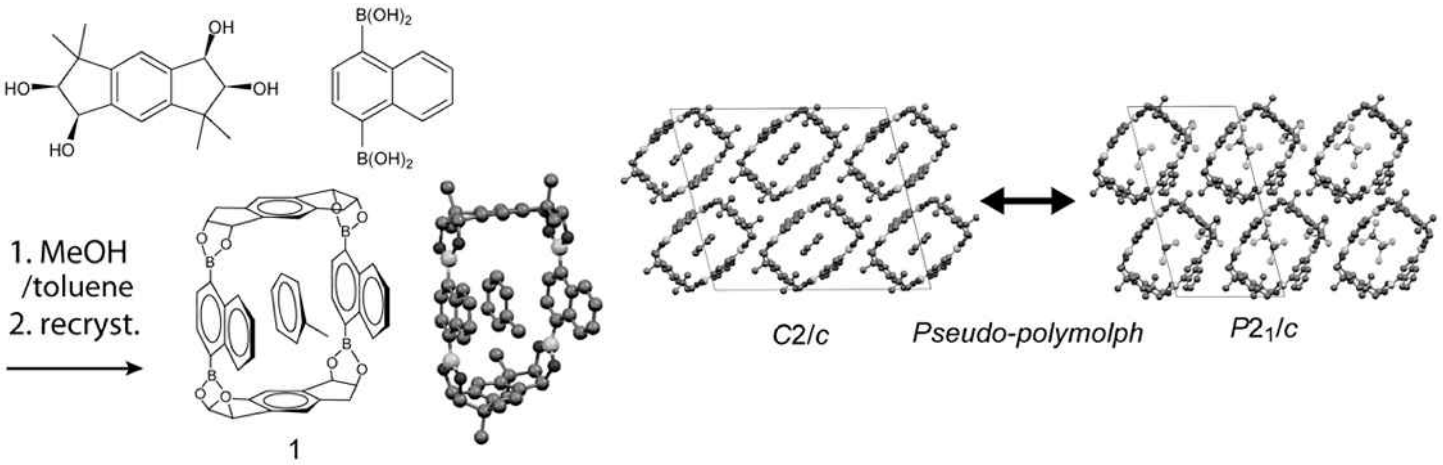
Macrocyclic compound has been attracting increasing attention because of their application for guest absorption and storage, guest selectivity, and reaction environment, which would utilize void space in the compound. Recently, such macrocyclic compound, boronic esters, has found to be formed as dynamic self-assembly of organic molecules through solvent dependent dynamic covalent bond formation between racemic polyol and planar 1,4-benzen(boronic acid)[1]. Thus, it is important to determine the crystal structure of the macrocyclic boronic esters with incorporated guest molecule to reveal the features of the compounds. In this study, structures of boronic ester of 1,4- naphthalene(boronic acid) (1) are presented and compared. The boronic ester with toluene guest molecule crystalized in monoclinic system, C2/c, Z=4, V=5099.7(6) Å3. As expected, toluene molecule was accommodated within a ring sandwiched by two naphthalene rings suggesting π-π interaction (ca. 3.6 Å separations). It is interesting that other structures of 1 with 1,4-dicyanobenzene, chloroform, and THF also have isomorphic structures to 1 with toluene. It clearly shows the guest inclusion ability of this boronic ester by weak intermolecular interactions. In the crystal structures, the boronic ester aligned along b-axis forming one-dimensional stacking with channel structure filled with guest molecules. Also, 1 with chloroform has a pseudo-polymorph phase (P21/c, V=5780.8(13) Å3) that has two additional chloroform molecules inside and outside of the ring; however, it also shows similar one-dimensional stacking structure with channel, implying this boronic ester has an easily stacking molecular shape. Although, the molecules have similar [2+2] ring structure, dihedral angle between two facing naphthalene rings is different in 1 with toluene, which is smaller as 14.1° than 22 to 24° in other structures. It may indicate a flexibility of the macrocyclic ring.

***[1]*** *N. Iwasawa, H. Takahagi, J. Am. Chem. Soc., 2007, 129, 7754-7755*

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