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Macrocyclic Boronic Ester: Porous and Host-Guest Structures Revealed by SDPD

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Diboronic acid and racemic tetrol are found to form a self-assembled macrocyclic boronic ester in the presence of appropriate guest molecules[1]. In the crystal, stacking of macrocyclic ring is observed to form infinite channel structure accommodating guest molecules by supramolecular interactions. In such structure, it is important to investigate the guest uptake and release mechanism via the crystal structure determination of the guest-free apohost. However, the apohost crystal can only be obtained by guest release process by heating, which results to form powder crystals. In this study, the structure of apohost was determined by "Structure Determination from Powder X-ray Diffraction data" technique [2][3] and the structural change by guest sorption and desorption processes were investigated. The powder X-ray diffraction pattern of the toluene inclusion crystal and the apohost crystal, which was obtained by heating of the inclusion crystal, are significantly different. However, even after the guest release, the apohost structure determined from the powder X-ray diffraction data was found to retain its crystal packing with one dimensional guest free channel. Interestingly, the apohost crystal easily absorbs the toluene and other aromatic molecules when the vapor was applied, and the crystal transforms into the guest inclusion crystal. Also, such vapor application is interesting method to switch the physicochemical property of the crystal. When naphthalene vapor was applied to the apohost crystal, naphthalene inclusion crystal was readily formed, and it became fluorescent crystal. This property was switched off by heating and guest desorption. In summary, the macrocyclic boronic ester is promising compound that forms inclusion supramolecular crystal, which can be utilized as guest storage / release, separate, protect, and other physicochemical functional material.

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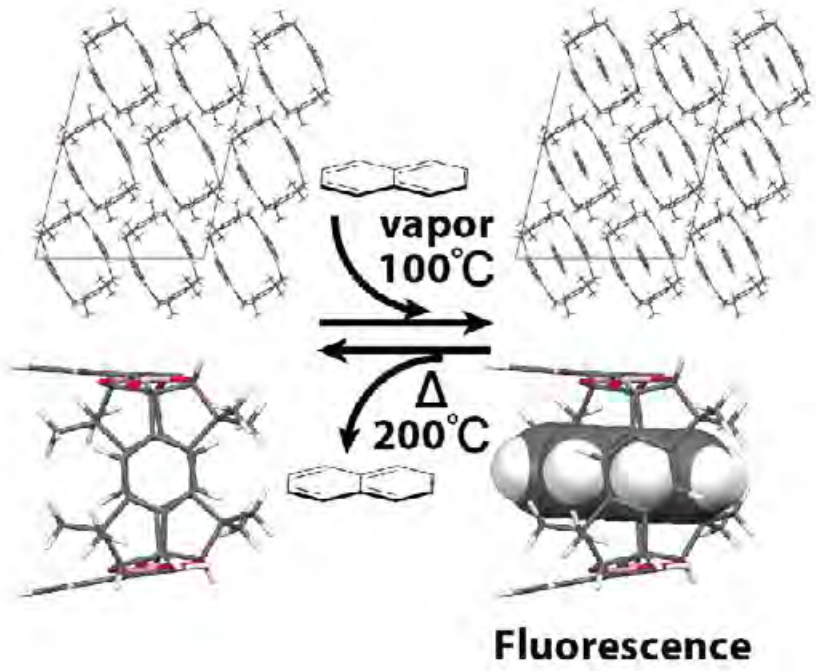

Keywords: Porous crystal, Structure Determination from Powder Diffraction data, host-guest interaction