

Poster Presentation

MS43.P19

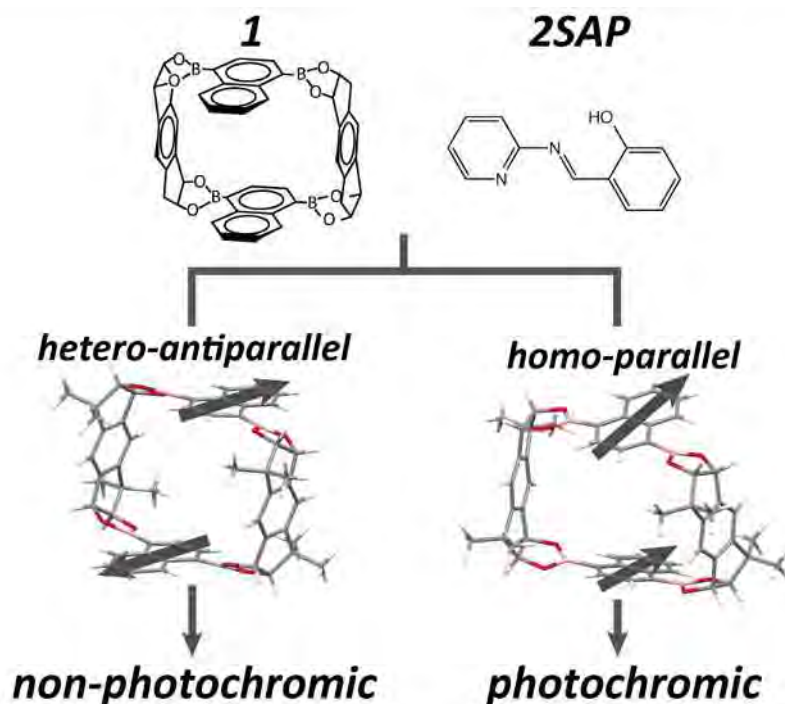
Photochromism change by conformation control in macrocyclic boronic ester cavity

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N-salicylideneaniline derivatives are known to show photochromism by UV light, and it depends on the molecular conformation in the crystal. The twisted molecule is photochromic but the planar one is not[1,2]. N-salicylidene-2-aminopyridine (2SAP) always has a planar conformation due to the chemical structure without steric hindrance, therefore 2SAP is known as non-photochromic. However, by confining the molecule in a cavity of the macrocyclic boronic ester **1**[3], the conformation and photochromism can be controlled. The inclusion crystal of **1** (homo-parallel form) has a special feature to have a channel type crystal structure in which the macrocyclic ring aligned one-dimensionally to include guest molecules. Interestingly, the crystals can reversibly absorb/desorb guests maintaining the crystal structure, because the channel structure is robust. To exchange the included guests, the crystal of **1**(homo-parallel form) was immersed in the melt of 2SAP at 90°C. The obtained inclusion crystal showed photochromism. In the crystal structure, the shape of residual electron density for 2SAP indicated the conformation of 2SAP was twisted due to the confining in the cavity, which is the reason for photochromism. On the other hand, the recrystallization of **1** and 2SAP from THF / hexane solution unexpectedly gave hetero-antiparallel form of **1** because of the dynamic covalent bond formation in the boronic esters (Fig.). As this hetero-antiparallel form has planar cavity in the molecule, the conformation of the included guest molecule, 2SAP, is also planar as always seen. Therefore the inclusion crystal is non-photochromic. Thus, photochromism change of 2SAP was realized by conformational control through confining in the cavity of macrocyclic boronic ester.

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Keywords: photochromism, salicylideneaniline, boronic ester