Creation of Luminescent Polymorphic Material Based on Chirality of Boron-Fused Azomethine Complex

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Keywords: Boron; Azomethine; Luminescence; Fused structure; Polymorph

Polymorphism alteration is currently recognized as a promising strategy to tune a crystalline-state emissive property and various types of optically-functional materials have been developed. However, precise controls of polymorphism are extensively challenging because it is difficult to predict whether a newly synthesized compound is polymorphic or not. To propose one solve for this problem, we focused on the stereogenic boron center of boron-fused azomethine (**BAm**) complex. In our previous research, we obtained the two polymorphs as racemic crystals consisting of (*R*)- and (*S*)-enantiomers of **BAm** with intense solid-state emission.[1)] From these results, we assumed that another luminescent homochiral crystal would be available by the chiral resolution. In this work, we synthesized a new **BAm** derivative with the chlorine substitution (**BAmCl**) and separated its enantiomers (Figure 1).[2)] As a result, we succeeded in obtaining the homochiral crystals of (*R*)- and (*S*)-**BAmCl** as well as the racemic crystal *rac*-**BAmCl**.

From the result of a single crystal X-ray diffraction (SCXRD) analysis, it was proposed that a variety of the intermolecular interactions and the intrinsic flexibility of **BAm** framework contributed to the stabilization of the homochiral crystal (Figure 2). Moreover, these two crystals showed different emission colors dependent on the molecular arrangements. Additionally, in the homochiral crystal, the homogeneous racemization was observed through the molten state in the absence of any solvents and catalysts. To the best of our knowledge, this is the first example of homogeneous racemization in the boron-centered chiral compounds.

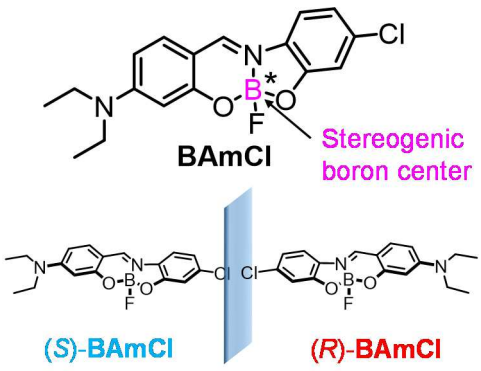

Figure 1. Chemical structure of **BAmCl** and its stereogenic boron center.

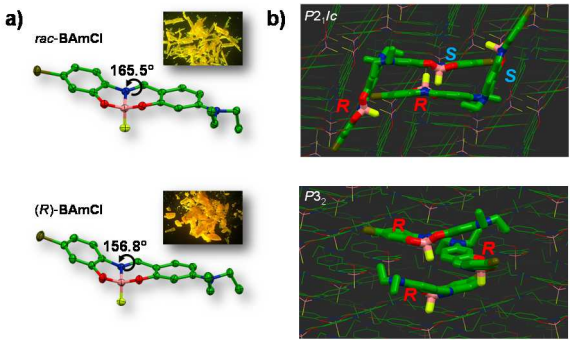

Figure 2. a) Thermal ellipsoid (probability level 50%) and b) packing structures of *rac*-**BAmCl** and (*R*)-**BAmCl** (*green* carbon atoms; *blue* nitrogen atoms; *red* oxygen atoms; *pink* boron atoms; *yellow* fluorine atoms; *gold* chlorine atoms; hydrogen atoms are omitted for clarity).

1) Ohtani, S.; Gon, M.; Tanaka, K.; Chujo, Y. *Chem. Eur. J.* **2017**, *23*, 11827.
2) Ohtani, S.; Takeda, Y.; Gon, M.; Tanaka, K.; Chujo, Y. *Chem. Commun.* **2020**, *56*, 15305.