

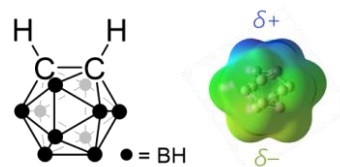
## Design of Solid-State Photoluminescence Materials Based on Stacked $\pi$ -Planes Assisted by Carborane

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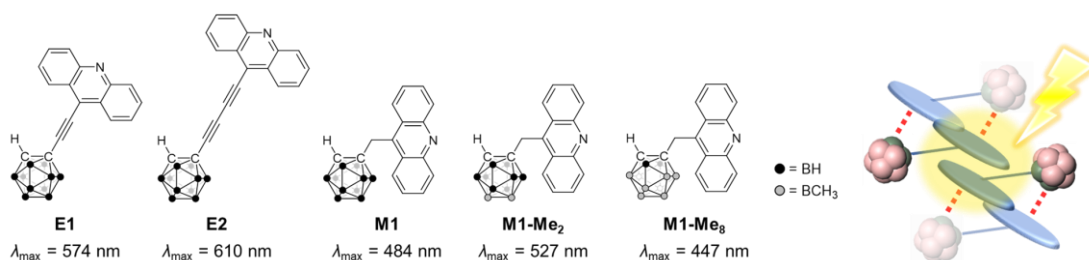
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*o*-Carborane is an icosahedral cluster composed of ten boron and two carbon atoms with three-center two-electron ( $3c2e$ ) bonds. Its three-dimensionally delocalized skeletal electrons through  $3c2e$  bonds can be an origin of various unique luminescent properties.<sup>[1]</sup> Moreover, the electronically polarized structure has the potential to form electrostatic interactions and therefore to be a versatile scaffold to develop functional materials (Fig. 1).



**Fig. 1** (left) Chemical structure of *o*-carborane. (right) Electrostatic potential map of *o*-carborane.

In this research, we synthesized five types of acridine-modified compounds (Fig. 2, left).<sup>[2]</sup> There are two types of classification: spacer units and methylation degree. First, **E1**, **E2**, and **M1** contain various spacer units with different conjugation length. Second, **M1**, **M1-Me<sub>2</sub>**, and **M1-Me<sub>8</sub>** have the same methylene spacer but different carborane skeletons with partial methylation. Interestingly, these five compounds showed a wide range of photoluminescence in the crystalline state from light blue to orange. After the series of measurements under various conditions, we attributed those broad emission bands to solid-state excimer emission derived from the  $\pi$ -stacking in the crystalline state. From single-crystal X-ray analyses, it was revealed that all compounds formed a dimer structure assisted by  $\text{CH}\cdots\text{N}$  interactions, and efficient  $\pi$ - $\pi$  interaction was formed (Fig. 2, right). It can be concluded that a slight change of  $\pi$ - $\pi$  interaction by chemical modifications drastically influenced the photoluminescence from the crystalline samples.



**Fig. 2** (left) The synthesized compounds. (right) Dimer structure assisted by  $\text{CH}\cdots\text{N}$  interactions.

1) J. Ochi, K. Tanaka, Y. Chujo. *Angew. Chem. Int. Ed.*, **2019**, 59, 9841–9855.

2) For **E1** and **E2**: J. Ochi, K. Tanaka, Y. Chujo. *Inorg. Chem.*, **2021**, 60, 8990–8997.