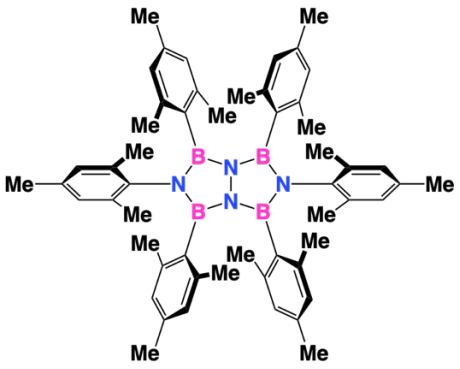
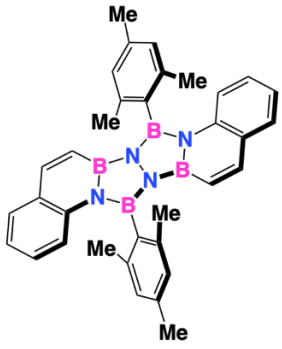
Synthesis, Properties, and π-Extension of B_4N_4-Heteropentalene Derivatives

([1]*Lab. Chem. Life Sci., Tokyo Tech.*, [2]*Sch. Mater. and Chem. Tech., Tokyo Tech.*)
○Junki Kashida[1,2], Yoshiaki Shoji[1,2], Takanori Fukushima[1,2]
Keywords: *BN-Containing π-Conjugated Molecule*; *Element Substitution*; *Pentalene*; *Phosphorescence*; *Host Material*

The replacement of C–C bonds of π-conjugated molecules with isoelectronic but polar B–N bonds can endow π-conjugated molecules with new electronic and optoelectronic properties. We recently showed that a 1,3,2,4-diazadiboretidine derivative, featuring a cyclic B_2N_2 four-membered ring with an isoelectronic structure of cyclobutadiene, displays blue phosphorescence in solution at room temperature.[1] Here we report the synthesis and properties of a B_4N_4-heteropentalene derivative (**1**).[2] Due to the steric protection by six mesityl groups, **1** showed remarkable stability toward air and even water. Single-crystal X-ray analysis of **1** revealed bonding characters of the B_4N_4-heteropentalene moiety. Compound **1** emits short-wavelength blue phosphorescence in a glassy matrix at 77 K, indicating that **1** has a high triplet energy. Motivated by this finding, we fabricated an OLED device using **1** and $Ir(ppy)_3$ as a host material and green phosphorescence emitter, respectively, where a relatively high external quantum efficiency (~15%) was achieved. In this presentation, we also report the synthesis and properties of a new π-extended B_4N_4-heteropentalene (**2**).



1



2

[1] Y. Shoji, Y. Ikabata, I. Ryzhii, R. Ayub, O. El Bakouri, T. Sato, Q. Wang, T. Miura, B. S. B. Karunathilaka, Y. Tsuchiya, C. Adachi, H. Ottosson, H. Nakai, T. Ikoma, T. Fukushima, *Angew. Chem. Int. Ed.,* **2021**, *60*, 21817–21823.

[2] J. Kashida, Y. Shoji, Y. Ikabata, H. Taka, H. Sakai, T. Hasobe, H. Nakai, T. Fukushima, *Angew. Chem. Int. Ed.,* **2021**, *60*, 23812–23818.