Regulation of the Optical Properties of Boron Tropolonate Complexes Based on Regioselective Substitution

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π-conjugated molecules have been developed in various fields such as organic light emitting diodes or sensors thanks to their luminescent and redox properties. In order to control these properties, regulating the frontier molecular orbital (FMO) energy levels plays an important role. In our laboratory, "Isolated FMO" was proposed as a feasible strategy to control HOMO and LUMO energy levels.[1] The position with only HOMO or LUMO distribution on the skeletal carbon is defined as "isolated HOMO" or "isolated LUMO." For example, FMO energy levels of **5AP** can be independently controlled by regioselective substitution of isolated HOMO or LUMO.[2] In common, molecules with isolated FMOs have even-electron/odd-atom (ee/oa) system, where even π-electrons are conjugated over odd atoms (Figure 1).

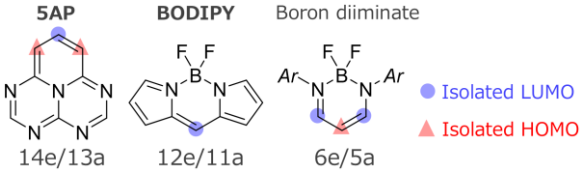

Figure 1. Molecules with isolated FMOs.

In this work, we developed a novel isolated FMO scaffold based on ee/oa system. As shown in Figure 2, **Tp** has conjugated system with 10 electrons on 9 atoms, *i.e.* two oxygen atoms and a seven-membered ring. It is reported that **TpB**, the simplest difluoroboron tropolonate complex, shows improved photoluminescence compared to **Tp**.[3] We introduced various substitutions on isolated HOMO of **TpB** to control the luminescent properties of **TpB** (Figure 3). It was revealed that the FMO energy levels and luminescent wavelength are tunable by the effect of substituents. In addition, advanced photophysical behavior such as room temperature phosphorescence or aggregation-induced emission was achieved.

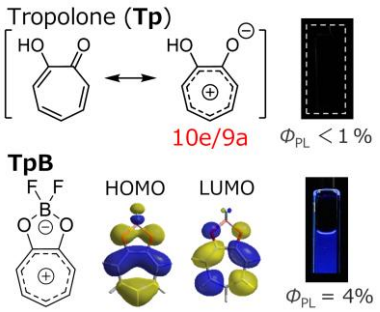

Figure 2. Tp and **TpB**.

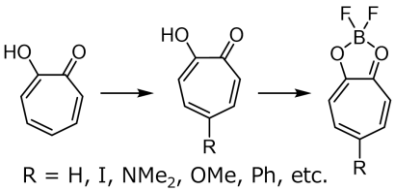

Figure 3. Chemical structures of synthesized compounds based on **Tp**.

1) K. Tanaka, *Polym. J.* **2024**, *56*, 61–70.
2) H. Watanabe, K. Tanaka, Y. Chujo, *Asian J. Org. Chem.* **2022**, *11*, e202200221.
3) H. Ogoshi, S. Ito, K. Tanaka, *Bull. Chem. Soc. Jpn.* **2023**, *96*, 452–460.