外周部位を環状アルキル骨格で保護したヘリセン誘導体の合成と光物性

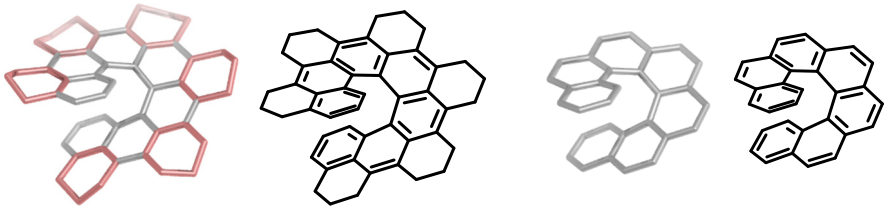
（京大化研[1]・JST さきがけ[2]）○志村 怜雄[1]・劉 之博[1]・廣瀬 崇至[1,2]

Peripheral Protection of [7]Helicene and its effects on the Photophysical Properties ([1]*Institute for Chemical Research, Kyoto University,* [2]*PRESTO, Japan Science and Technology Agency*)
○Reo Shimura,[1] Zhibo Liu,[1] Takashi Hirose[1,2]

Helical polycyclic aromatic hydrocarbons (HPAHs) are expected to exhibit strong circular dichroism (CD) and circularly polarized luminescence (CPL) because of their helically-twisted electronic structures.[1] In terms of the application of chiral emitters, chemically stable chiral luminophores are required to create circularly-polarized organic light-emitting devices (CP-OLEDs).[2] In order to develop the molecular structure of chiral emitters that exhibit good luminescence properties in the solid state, it is necessary to elucidate the excited state dynamics in the solid state and their electronic interactions between the chiral emitter and the solid matrix. In this work, we focused on a [7]helicene derivative with partially saturated six-membered rings consisting of propylene group fused to the outer moiety of the helically twisted π-conjugated core, which was prepared according to the previously reported synthetic method.[3] In this presentation, the effect of protecting the helical π-conjugated core with a cyclic alkyl skeleton on the luminescence properties will be discussed in detail.

Keywords : Emission Properties; Chirality; Cyclic Alkyl Flamework; Helicenes

らせん状の歪みを持つ多環芳香族炭化水素 (HPAHs) は、らせん状に捻じれた分子軌道に由来して、良好な円二色性 (CD) および円偏光発光 (CPL) 特性を示すことが期待される [1,2]。固体状態で良好な発光特性を示すキラル発光体の分子構造を開拓するためには、固体状態におけるキラル発光色素の電子状態と励起状態ダイナミクスを解明する必要がある。本研究では、外周部位に部分的に飽和した六員環を縮環した[7]ヘリセン誘導体 (**1**) のユニークな分子構造に着目し [3]、その光物性を調査することを目的とした。本発表では、らせん状の π 共役コアを環状アルキル骨格で保護した場合の発光特性への影響について量子化学計算の結果を踏まえて詳細に議論する。



1) Y. Shen, C.-F. Chen, *Chem. Rev.* **2012**, *112*, 1463. 2) D.-W. Zhang, M. Li, C.-F. Chen, *Chem. Soc. Rev.* **2020**, *49*, 1331. 3) Y. Nakakuki, T. Hirose, H. Sotome, H. Miyasaka, K. Matsuda, *J. Am. Chem. Soc.* **2018**, *140*, 4317.