

Encapsulation of Stacked Antiaromatic Norcorrole Ni(II) Complexes in a Water-Soluble Micellar Capsule

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The interaction between two stacked antiaromatic π -systems has recently attracted considerable attention. Our group reported that norcorrole, which is an antiaromatic porphyrinoid, tends to form a face-to-face stacked dimer with a remarkably short interplanar distance ($< 3.4 \text{ \AA}$), leading to effective orbital interaction. The remarkable proximity of the two norcorrole units has been rationalized by the emergence of stacked-ring aromaticity. However, the current strategy to achieve stacked-ring aromaticity consists only of the tethering approach, which requires the elaborate synthesis of norcorrole dimers.¹

Here, we demonstrate the realization of stacked-ring aromaticity by a rational supramolecular approach. Several norcorrole Ni(II) complexes were subjected to the encapsulation in a micellar capsule composed of bent polyaromatic amphiphiles.² The encapsulation resulted in the appearance of a broad absorption band in the near infrared region, which is characteristic of face-to-face stacked norcorrole dimers. Importantly, 5,15-diisopropylnorcorrole, which does not exhibit π -stacked orientation even in a concentrated organic solvent and crystalline phase, adopted π -stacking in the micellar capsule. These results demonstrate the power of supramolecular chemistry for the realization of stacked-ring aromaticity.



- 1) a) R. Nozawa, H. Tanaka, W.-Y. Cha, Y. Hong, I. Hisaki, S. Shimizu, J.-Y. Shin, T. Kowalczyk, S. Irle, D. Kim, H. Shinokubo, *Nat. Commun.* **2016**, 7, 13620. b) R. Nozawa, J. Kim, J. Oh, A. Lamping, Y. Wang, S. Shimizu, I. Hisaki, T. Kowalczyk, H. Fliegl, D. Kim, H. Shinokubo, *Nat. Commun.* **2019**, 10, 3576.
- 2) K. Kondo, A. Suzuki, M. Akita, M. Yoshizawa, *Angew. Chem. Int. Ed.* **2013**, 52, 2308.