Cyclic Bifluorenylidene Trimer: Relationship between Dynamic Behaviors and Structural Characteristics

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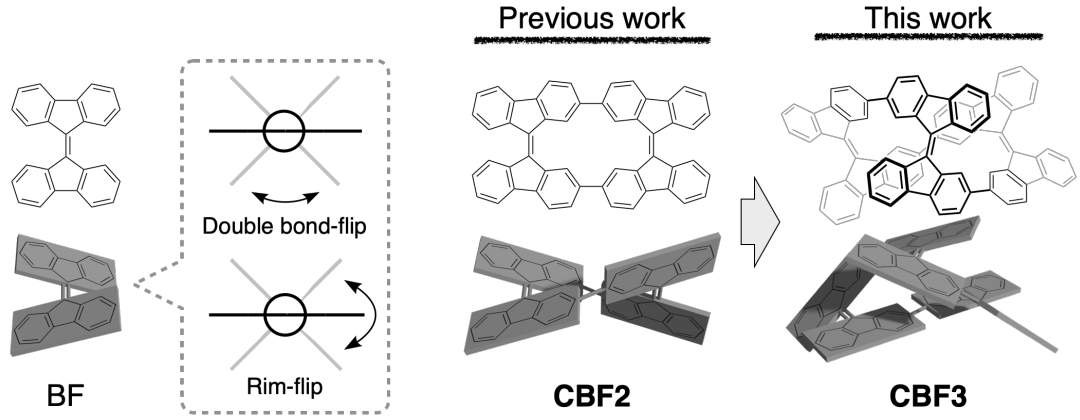
Many molecules mimicking macroscopic machines, such as rotors, gears, and so forth, have been synthesized.[1] However, they occasionally cannot transfer the motion due to an unexpected motion.[2] Exploiting molecular units enabling infallible motion transmission is an important issue in constructing molecular machines. As a dynamic unit of molecular machine, we chose 9,9'-bifluorenylidene (BF), one of the polyaromatic hydrocarbons having a thermally isomerizable C=C double bond via rim-flip and double bond-flip mechanism.[3] In our previous research, we synthesized the cyclic dimer of BF (**CBF2**) that only showed the rim-flipping motion. [4]

In this research, we synthesized a cyclic trimer (**CBF3**) which is supposed to isomerize both via rim-flip and double bond-flip mechanism. Since **CBF3** has a chirality derived from its twisted structure, the optical resolution of **CBF3** was performed; the chiroptical property of **CBF3** indicates that the racemization of **CBF3** occurs thermally at room temperature. The racemization mechanism was proposed through the ^{1}H EXSY measurement and DFT calculation. The characteristic of this mechanism is that three double bonds in **CBF3** are isomerized in a continuous fashion. This result, the interlocking motion of several movable points, is of importance in the field relating to molecular machines.



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