

# Three-Dimensional $\pi$ -Electron Molecules

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Organic molecules possessing three-dimensional (3D) curved  $\pi$ -conjugated structures are attractive research targets in organic synthesis, physical organic chemistry, and organic material science. Our research interest is the creation of new 3D  $\pi$ -conjugated organic molecules, the elucidation of properties, and the application in material science.

## 1. Acid/Base-Responsive Helicenes

We discovered a new phenomenon that N–N linked helical bicarbazole (BC) and tetramethylbiacridine (TBA) derivatives undergo reversible electron transfer disproportionation by acid/base stimuli with contrast photophysical and magnetic properties.<sup>1)</sup> The reaction goes through an acid-triggered homolytic N–N bond cleavage reaction of BC or TBA.

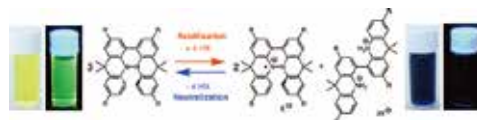


Figure 1. Acid/base-regulated electron transfer disproportionation.

## 2. Thermal Dynamics of Buckybowls

Buckybowls, bowl-shaped aromatic compounds, have a unique thermal dynamic behavior, *i.e.* bowl inversion. Thermal dynamics of a buckybowl dimer, bisumanenyl, was studied and elucidated by combination of NMR experiment and DFT calculation.<sup>2)</sup>

### References

- 1) P. Pandit, K. Yamamoto, T. Nakamura, K. Nishimura, Y. Kurashige, T. Yanai, G. Nakamura, S. Masaoka, K. Furukawa, Y. Yakiyama, M. Kawano and S. Higashibayashi, *Chem. Sci.* **6**, 4160–4173 (2015).
- 2) B. B. Shrestha, S. Karanjit, S. Higashibayashi, T. Amaya, T. Hirao and H. Sakurai, *Asian J. Org. Chem.* **4**, 62–68 (2015).