

ジベンゾ[g,p]クリセンの非平面性を制御する置換反応の開発

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Relevant Synthesis to Manipulating Non-Planarity in Dibenzo[g,p]chrysene: Substitution Reactions at the Bay (Ryukoku University) ○Naruhiro Yoshida, Ryuhei Akasaka, Tetsuo Iwasawa

Manipulating the non-planarity of pi-conjugated molecules is significant for the development of functional organic materials those underpin our future technologies. Because the effect of the twist on molecular packing that involves orbital interactions clearly appears in solid state properties such as carrier transportation. Among such types of non-planar pi-systems, dibenzo[g,p]chrysene (DBC) is known as one of the most appealing polyaromatic hydrocarbons. We chemists have long sought to develop DBC derivatives; however, synthetic problems prevent us to deploy DBCs as not only molecular materials but also basic research target compounds. Herein we present to perform substitution reactions at four bromines of the bay regions. With the aid of DFT computational procedures as well as crystallographic data, DBCs turned out to be flexibly movable in a range of about 26°. In addition, several kinds of chemical properties in DBC cores were also unveiled (Figure 1).

Keywords : Arenes; Dibenzo[g,p]chrysene; Non-planar pi-conjugation; Polycycles; Torsion angles

組成式 $C_{26}H_{16}$ のジベンゾ[g,p]クリセン (以下、DBC) は、六環性の比較的小さな非平面性の π 共役系を有する縮環分子である。典型的な多環芳香族炭化水素であるが、どのくらいのねじれ角を持って歪むのか、また、それに伴ってどのくらいの変化をもって物性が異なるのか、基本的なことがよくわかっていない。今回我々は、液相条件下で取扱可能な DBC のベイ領域にさまざまな置換基を導入して、どのくらいの範囲でねじれ角が動くのか、定量的に評価する実験研究に臨んだ。その結果、ねじれ角が最大で 57 度・最小で 31 度の範囲で変化することを、X 線構造解析と DFT 計算を用いて、明らかにした¹⁾。

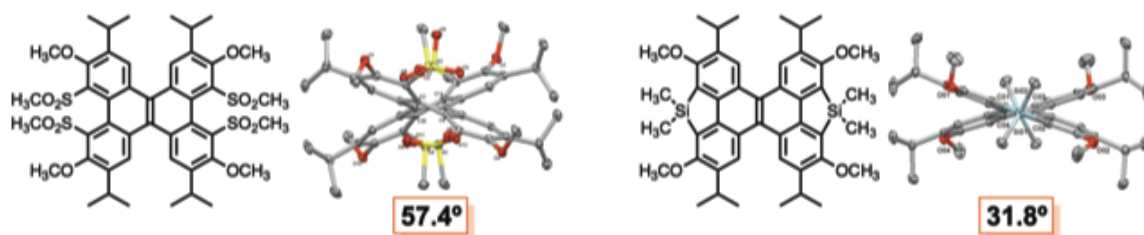


Figure 1. With the aid of DFT calculations and crystallographic analyses, the DBC core turned out to be flexibly movable in a range of from 57° to 31°.

- 1) S. Kamiguchi, R. Akasaka, N. Yoshida, T. Imai, Y. Yamaoka, T. Amaya, T. Iwasawa, *Tetrahedron Lett.* **2022**, 92, 153664.