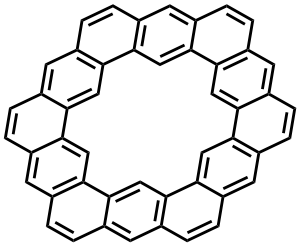
８の字形立体ねじれ構造をもつ多環芳香族炭化水素インフィニテンの合成と物性

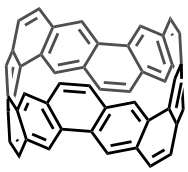
（名大院理[1]・名大 WPI-ITbM[2]）○伊藤 英人[1]・Krzeszewski Maciej[1]・伊丹 健一郎[1,2]
Infinitene: A Helically Twisted Figure-Eight [12]Circulene Topoisomer ([1]*Graduate School of Science, Nagoya University*, [2]*Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University*) ○Hideto Ito,[1] Krzeszewski Maciej,[1] Kenichiro Itami[1,2]

Kekulene[1] is one of polycyclic aromatic hydrocarbons (PAHs) having a molecular formula of $C_{48}H_{24}$, and also represents a topoisomer of [6,6]carbon nanobelt[2] and yet-unsynthesized [12]circulene.[2] These "$C_{48}H_{24}$ molecules" are expected to have various interesting properties depending on their fused structures and circular shapes. As one of other possible circular topoisomers of $C_{48}H_{24}$, a helically twisted figure-eight PAH[3] would theoretically exist, and we named this simple and beautiful molecule as "infinitene". In this study, we succeeded to synthesize infinitene as a novel topoisomer of $C_{48}H_{24}$.[4] Unlike kekulene, [6,6]carbon nanobelt and [12]circulene, infinitene has an intrinsic molecular chirality derived from two helicene moieties, and both *P*,*P*- and *M*,*M*-enantiomers could be resolved by HPLC with a chiral column. In the presentation, we will present the synthesis, structural features, and photophysical and chiroptical properties of infinitene.
Keywords: Polycyclic aromatic hydrocarbon; circulene; kekulene; Ladder molecule; helicene

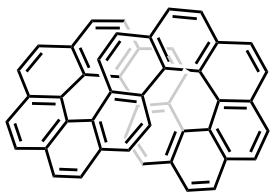
$C_{48}H_{24}$ の分子式をもつ多環芳香族炭化水素（PAH）には kekulene[1]、[6,6]カーボンナノベルト[2]や未合成の[12]circulene などがあり、それぞれ縮環様式や環状構造の違いによって多種多様な物性を示すため興味深い。今回我々は、$C_{48}H_{24}$ の新たな環状トポ異性体の一つであり、８の字形で立体的にねじれたシンプルで美しい PAH[3]、「infinitene（インフィニテン）」の合成に成功した[4]。Infinitene は kekulene や[6,6]カーボンナノベルトとは異なり、２つのヘリセン部分構造に基づくねじれ構造による分子不斉を有しており、エナンチオマーが存在する。発表では infinitene の合成、構造、光物性や、エナンチオマーの光学分割、キラル光学特性などについて報告する。



Kekulene[1] ($C_{48}H_{24}$)



[6,6]Carbon nanobelt[2] ($C_{48}H_{24}$)



Infinitene[4] ($C_{48}H_{24}$)

[This work]

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