

学位論文の要旨

Abstract of Thesis

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学位論文題目 Title of Thesis (学位論文題目が英語の場合は和訳を付記)

Synthesis and Physicochemical Properties of Substituted Picenes
(置換ピセンの合成と物理化学的性質)

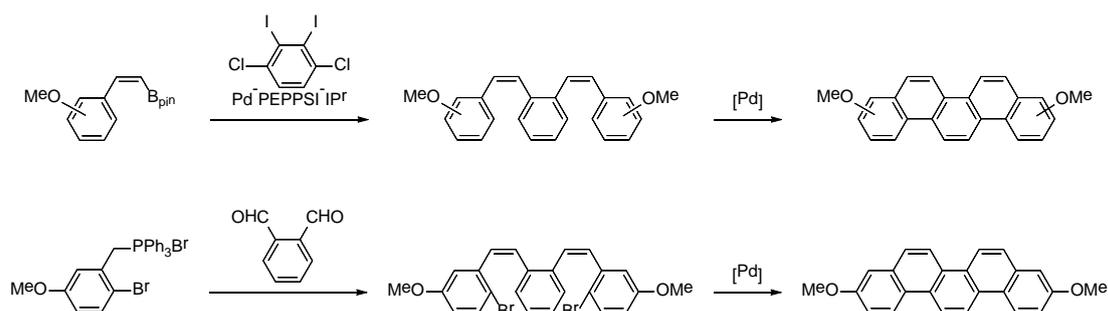
学位論文の要旨 Abstract of Thesis

A research of organic field-effect transistors (OFETs) has gained significant interest because of their high potential for use as organic electronic devices that possess advantageous features such as flexibility, lightweight, large-area coverage, ambipolar property, and low-cost/low-temperature fabrication process. Toward the development of OFETs, various organic materials have been designed and synthesized. Fused aromatic compounds containing π -conjugated systems are notable for their utility in organic field-effect transistors. Among them, picene ([5]phenacene) is a promising class of materials for OFETs, because it is an air-stable compound originating from its large band gap and higher ionization potential. Despite the promising properties of picene and its derivatives toward OFETs, the utilization for the device fabrication was limited due to inefficient synthetic route. Recently, the author's group reported an efficient synthetic method for the synthesis of various kinds of substituted picenes through Suzuki-Miyaura cross-coupling and sequential intramolecular double cyclization sequence *via* C-H bond activation.

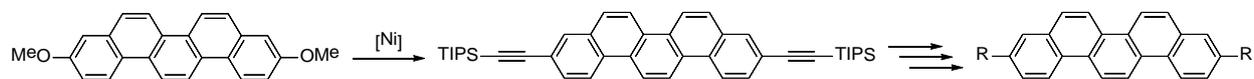
Chapter 1 describes the research background of OFETs (organic field-effect transistors), development of OFETs based on [n]phenacenes, and representative recent synthetic methods of [n]phenacenes. Accordingly, the new synthetic methodology of substituted picenes have been proposed.

Chapter 2 describes the synthesis of various methoxy-substituted picenes through Suzuki-Miyaura

cross-coupling and cyclization reactions. Although methoxypicenes substituted at 1,12-, 2,4,9,11-, 2,11-, 4,9-positions could be successfully synthesized, no 3,10-dimethoxypicene was formed. In order to synthesize 3,10-dimethoxypicene Wittig reaction and the palladium-catalyzed intramolecular cyclization *via* C-H bond activation was exploited. According to the comparison for the single crystals of these four methoxy-substituted picenes, it is found that the packing structure of 3,10-dimethoxypicene was 3D-Herringbone structure and that the crystal structures of these picenes strongly depend on their substitution position and the number of methoxy groups. The methoxy picenes have less effective intermolecular overlaps than that of picene, and the intermolecular electronic coupling depends on their packing structures and/or HOMO distribution. This property shows that 3,10-dimethoxypicene is supposed to show the best hole mobility. Despite the promising properties of 3,10-dimethoxypicene toward OFETs, its poor solubility in organic solvent limited its utilization for device fabrication by a solution process, which is desired for application in organic electronic devices.



In **Chapter 3**, some linear alkyl chains have been introduced into the parent picene. In order to make the derivatization of alkylated picenes more easily, the alkyl chains were introduced at the late stage. Ni-catalyzed alkylation of 3,10-dimethoxypicene *via* C-O bond activation resulted in the formation of 3,10-dialkylpicene. Then the subsequent desilylation, alkylation and hydrogenation sequences afforded a series of alkylpicenes in a divergent manner. The solubility of these alkylated picenes has also been elucidated. The solubility of picenes with longer alkyl chains up to 14 increased, whereas it was decreased as the carbon number increased more than 10. It is suggested that this results should be due to the hydrophobic interaction between the alkyl chains, which typically enhance an intermolecular interaction, leading to the low solubility.



Chapter 4 summarizes all the researches of this Thesis and demonstrates prospects related to this research field.

