異種の末端を有したジチアルビセン誘導体の合成と物性評価

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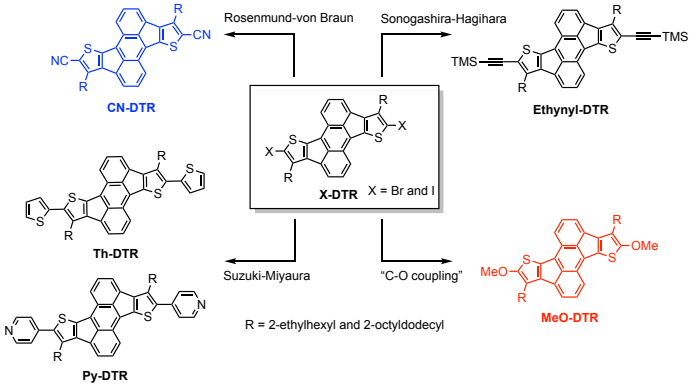
End-Functionalization of Dithiarubicene: Modulation of Optoelectronic Properties by Metal-Catalyzed Coupling Reactions ([1]*Graduate School of Engineering, Nagoya Institute of Technology,* [2]*The Institute of Scientific and Industrial Research (ISIR), Osaka University*) ○ Kenji Tsukamoto,[1] Koji Takagi,[1] Yutaka Ie,[2]

In order to modulate optoelectronic properties of dithiarubicene (**DTR**) by the end-functionalization and reveal the structure-properties relationship in detail, we have carried out a set of metal-catalyzed coupling reactions. Electron-withdrawing cyano (**CN-DTR**) and pyridyl (**Py-DTR**) groups, electron-donating methoxy (**MeO-DTR**) and thienyl (**Th-DTR**) groups, and relatively electron-neutral trimethylsilylethynyl (**Ethynyl-DTR**) group were introduced on the DTR core by using halogenated DTR derivatives as a precursor. Particularly, we could successfully install the methoxy group by the CuO-catalyzed reaction in high yield. As a result of the combination of electron-accepting DTR core and electron-donating methoxy group, UV-Vis absorption spectrum of **MeO-DTR** showed a large red-shift of the peak maximum by approximately 90 nm. In addition, the introduction of substituents made it possible to finely tune the HOMO and LUMO energy levels of DTR enabling the application in OFET devices. Thanks to the elevated HOMO energy level, the OFET device based on **MeO-DTR** exhibited a hole mobility (μ_h) up to 8.4×10^{-4} $cm^2 \cdot V^{-1} \cdot s^{-1}$. On the other hand, the device based on **CN-DTR** had an ambipolar characteristic, which exhibited a moderate electron mobility ($\mu_e = 1.1 \times 10^{-3}$ $cm^2 \cdot V^{-1} \cdot s^{-1}$) due to its low-lying LUMO energy level. From the XRD measurement, **MeO-DTR** and **CN-DTR** were found to show an edge-on molecular orientation on the HMDS-treated SiO_2 substrate.

Keywords : π-Conjugated Molecules; End-Functionalization; Metal-Catalyzed Coupling Reaction; Electron-accepting Core; Organic Semiconductor

ジチアルビセン(DTR)は、低い LUMO エネルギー準位および広範囲に及ぶ可視光吸収特性を有することから、OFET や OPV などの有機半導体材料として応用が期待される。しかし、現時点においてジチアルビセンを機能化する化学修飾の手法は極めて限られたものしか報告されていない。本研究では、ハロゲン化した DTR に対し金属カップリング反応を用いることで電子的性質の異なるさまざまな置換基を導入し、それらの HOMO/LUMO エネルギー準位やバンドギャップを精密に調整した化合物群を合成した。実際に、これらの化合物を用いて OFET 素子を作製したところ、輸送するキャリアに違いが観測された。



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