Control of Electron Correlation in Molecular Conductors by Difference of Stereochemistry

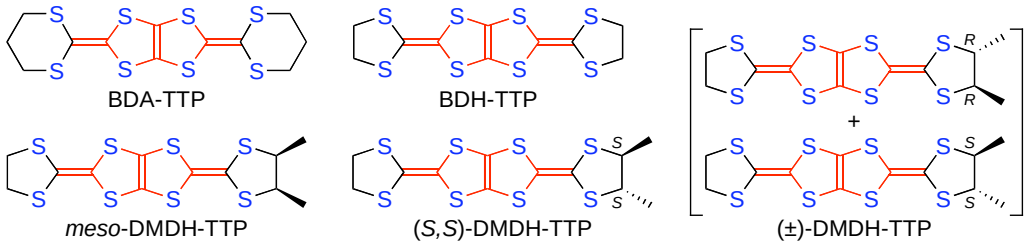
Kouki Miura[1], Satoshi Shimono[1], Hiroki Akutsu[1], Shin'ichi Nakatsuji[1], Jun-ichi Yamada[1], and Koichi Kikuchi[2]

[1]*Department of Material Science, University of Hyogo, Japan*

[2]*Department of Chemistry, Tokyo Metropolitan University, Japan*

Email: correspondence-yamada@sci.u-hyogo.ac.jp

Chemical modifications to π-electron donors used for the construction of molecular conductors lead to variations in the electron correlation (*U*/*W*, *U*, the on-site Coulomb repulsion, *W*, the bandwidth). We have found a series of BDA-TTP superconductors, and the molecular design of BDA-TTP is based on destabilization of the stable metallic state that occurs with the use of BDH-TTP [1]. Compared to the rigid outer dithiolane rings of BDH-TTP, BDA-TTP has more expanded outer dithiane rings capable of adopting various kinds of chair conformations. Such a chemical modification by extension of σ-framework would cause steric hindrance to intermolecular interaction and, consequently, would bring about a decrease in the bandwidth (*W*). An alternative chemical modification in this respect is to append alkyl substituents to the BDH-TTP skeleton; however, the attachment of an alkyl substituent to the respective carbon atoms on the ethylene end group of BDH-TTP results in chiral carbon centers. Therefore, we have begun to reveal the effect of the difference of stereochemistry in donor molecules on the electron correlation in molecular conductors. In this paper, we present the preparation, crystal structures, and conductivity of the *meso*-DMDH-TTP [2], (*S*,*S*)-DMDH-TTP, and (±)-DMDH-TTP salts.



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[2] J. Yamada *et al.*, *Chem. Lett.*, 34, 1404–1405 (2005); *Multifunctional Conducting Molecular Materials*, RSC Publishing, 63–66 (2007).