Structures and Properties of Molecular Conductors Based on and CHTM-TTP and Its Analogues

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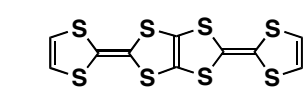
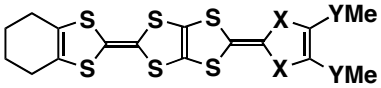
Bis-fused TTF (BDT-TTP) is of interest as a promising π-electron framework for the development of molecular conductors, because BDT-TTP and its derivatives have afforded many molecular metals stable down to low temperature. In this symposium, we report structures and properties of molecular conductors based on CHTM-TTP and its selenium analogues CHSM-TTP and CHTM-TS-TTP.

Figures 1 and 2 show crystal structures of (CHTM-TTP)$GaCl_4$ and (CHSM-TTP)AsF_6(PhCl), respectively. In the both materials, the fully oxidized donors are dimerized in the stacks. The calculations of overlap integrals and band structures suggest that there is no significant interstack interaction and that they are highly one-dimensional band insulators as a result. Electrical conductivity measurement revealed that both salts are actually semiconductirs. It is noted that (CHTM-TTP)$GaCl_4$ exhibits high conductivity of σ_{rt} = 2.9 S cm^{-1} with a low activation energy of 0.04 eV in spite of 1:1 salt.



BDT-TTP



X = Y = S, CHTM-TTP
X = S, Y = Se, CHSM-TTP
X = Se, Y = S, CHTM-TS-TTP

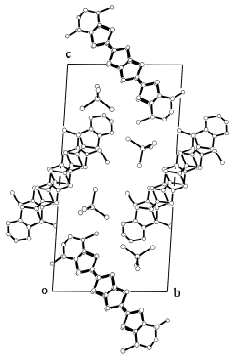


Fig. 1. Crystal structure of (CHTM-TTP)$GaCl_4$

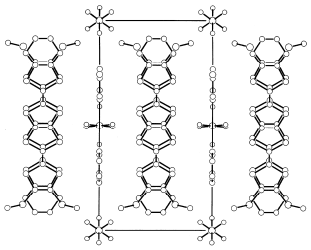


Fig. 2. Crystal structure of (CHSM-TTP)$AsF_6(C_6H_5Cl)$

* We are grateful to Drs. Hengbo Cui, Kazuyuki Takahashi and Prof. Hayao Kobayashi for kind assistance for X-ray structure analysis by using Rigaku AFC-8R Mercury CCD system at IMS.