

Incommensurate Structure of the Organic Superconductor (MDT-TS) $I_{0.85}Br_{0.41}$

Tadashi KAWAMOTO^{*}, Yoshimasa BANDO¹, Takehiko MORI¹, Toru KAKIUCHI², Hiroshi SAWA^{2,3}, Kazuo TAKIMIYA⁴, Tetsuo OTSUBO⁴

¹Department of Organic and Polymeric Materials, Graduate School of Science and Engineering, Tokyo Institute of Technology, O-okayama, Meguro-ku, Tokyo 152-8552, Japan

²Department of Materials Structure Science, The Graduate University of Advanced Studies, Tsukuba, Ibaraki 305-0801, Japan

³Institute of Materials Structure Science, High Energy of Accelerator Research Organization, Tsukuba, Ibaraki 305-0801, Japan

⁴Department of Applied Chemistry, Graduate School of Engineering, Hiroshima University, Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8527, Japan

Introduction

In organic superconductors, the ratios of the donor molecules to anions are represented by an integer (typically 2:1) [1]. By contrast, the MDT-TSF (methylenedithio-tetraselenafulvalene) series salts are incommensurate ambient pressure organic superconductors and the charge transfer degrees deviate from 0.5 [2]. Moreover, (MDT-TSF)(AuI₂)_{0.436} has shown the characteristic Fermi surface reconstruction by an incommensurate anion potential [3]. (MDT-TS)(AuI₂)_{0.441}, where MDT-TS is 5*H*-2-(1,3-diselenol-2-ylidene)-1,3,4,6-tetrathiapentalene, shows a metal-insulator transition at $T_{MI} = 50$ K in spite of the basically same crystal structure as those of the MDT-TSF superconductors [4]. The ground state of this salt changes from an “incommensurate antiferromagnetic insulating state” with $T_N = 50$ K to a superconducting phase at 3.2 K under 10.5 kbar [5]. We have discovered new organic conductor based on MDT-TS and I_xBr_y. The new conductor shows superconducting phase transition under high pressure. The present paper reports the incommensurate lattice structure of (MDT-TS) $I_{0.85}Br_{0.41}$.

Results and Discussion

Figure 1 shows the synchrotron radiation x-ray oscillation photograph at room temperature. This photograph clearly displays incommensurate layer lines. We distinguish the donor lattice and the anion lattice by indices h and h' , respectively. In Fig. 1, there are several spots around $h = 0$ line. These spots are originated in the convolution between $h = 1$ and $h' = 3$ lines. Although there is no clear spot at $h'=1$ line which comes from the length of I₃⁻ or I₂Br⁻, the Raman spectra show that the anion has a unit of I₃⁻. Therefore, the anions exist as trihalide anion chains composed by I and Br. The ratio between the length of the a -axes (a/a') is 1.2612(2) from Fig. 1, and the composition is estimated as (MDT-TS) $I_{0.85}Br_{0.41}$ from the x-ray oscillation photograph and the energy dispersion spectroscopy. This composition means that the MDT-TS molecule does not make a simple I₂Br or IBr₂ salt. We can speculate that the charge transfer degree

is 0.420 under assuming tri-halide anions. This value lies in between (MDT-TS)(AuI₂)_{0.441} and (MDT-TS)(I₃)_{0.407}. This result indicates that we can control the charge transfer degree (band-filling) in organic conductors based on MDT-TS with linear anions by changing the length of the anion.

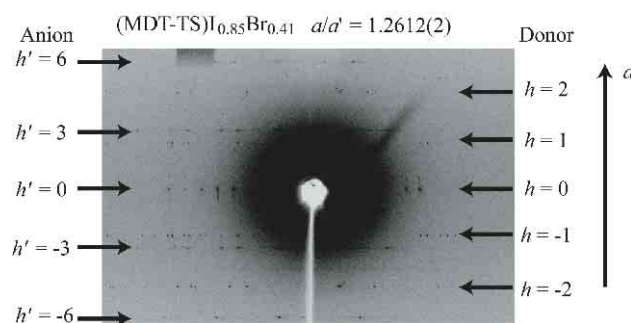


Figure 1: X-ray oscillation photograph. The vertical direction is along the donor stacking direction.

References

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* kawamoto@o.cc.titech.ac.jp