

Structural properties of the organic superconductor $\kappa_{\text{H}}\text{-(DMEDO-TSeF)}_2[\text{Au}(\text{CN})_4](\text{THF})$

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Introduction

Most organic superconductors have been obtained as clean single crystals; the donor molecules and anions are ordered states. Recently, two new organic superconductors with the same chemical composition, κ_{L} - and κ_{H} -(DMEDO-TSeF)₂[Au(CN)₄](THF), have been developed [1]. Although the solvent molecule THF of the high- T_c (H) phase is ordered even at room temperature, THF of the low- T_c (L) phase is disordered by the mirror symmetry. We have determined the structural phase transition in the L-phase; the orthorhombic system changes to two monoclinic domains below 209 K [2]. On the other hand, the H-phase has two crystallographically independent conducting layers, A and B. The quantum oscillation of this salt indicates that the interlayer charge disproportionation, where the difference charge is 0.05 degree, occurs despite of a bulk single crystal [3]. The present paper reports the low-temperature crystal structure of the H-phase.

Results and Discussion

The space group is $P2_1/c$, and the lattice parameters at 34 K are $a = 38.583(1)$ Å, $b = 10.9621(3)$ Å, $c = 8.1480(4)$ Å, $\beta = 93.626(5)^\circ$, and $V = 3439.3(2)$ Å³. The final R -value is $R1 = 0.069$.

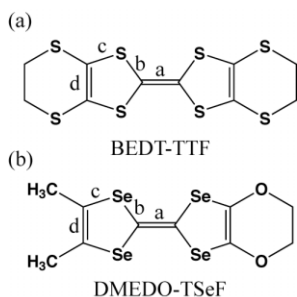


Figure 1: Labeling of the C-S (Se) and C=C averaged central bond lengths in (a) BEDT-TTF and (b) DMEDO-TSeF.

A method for determining experimentally the charges of the BEDT-TTF molecules has been developed using the intramolecular bond lengths [4-6]. Oxidation of the BEDT-TTF molecule lengthens a and d (C=C bonds), and shortens b and c (C-S bonds) as shown in Fig. 1(a). The parameter defined as $\delta = (b + c) - (a + d)$ is sensitive to the charge transfer degree of the BEDT-TTF molecule. The parameter δ decreases as the charge transfer degree increases. We should use this method for the present compound on the assumption of the D_{2h} symmetry for the tetraselenafulvalene unit of the DMEDO-TSeF molecule as shown in Fig. 1(b).

The bond lengths defined in Fig. 1(b) of the H-phase at 34 K are listed in Table I.

Table I. Intramolecular bond lengths of DMEDO-TSeF molecules, A and B, of the H-phase at 34 K.

	a (Å)	b (Å)	c (Å)	d (Å)
Molecule A	1.363(8)	1.888(3)	1.897(3)	1.345(6)
Molecule B	1.361(8)	1.888(3)	1.894(3)	1.350(6)

The parameter δ estimated from Table I is 1.08(1) for the A molecule, and is 1.07(1) for the B molecule, respectively. Therefore, we cannot distinguish the difference of the charge between of the A and the B molecules from the bond lengths. This result indicates that the bond lengths are not useful to clarify the interlayer charge disproportionation for the present compound. However, the resonant x-ray scattering method will be a powerful tool for this compound.

References

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