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Structural Phase Transition of the Organic Superconductor κ_L-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF)

Tadashi KAWAMOTO*[1], Takehiko MORI[2], Toru KAKIUCHI[3], Hiroshi SAWA[3,4], Takashi SHIRAHATA[5], Megumi KIBUNE[5], Hiroko YOSHINO[5], Tatsuro IMAKUBO[5]

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

[2]Department of Chemistry and Materials Science, Graduate School of Science and Engineering, Tokyo Institute of Technology, O-okayama, Meguro-ku, Tokyo 152-8552, Japan

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

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

[5]Imakubo Initiative Research Unit, RIKEN, Hirosawa, Wako, Saitama 351-0198, Japan

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. The present paper reports the structural phase transition of the L-phase; the orthorhombic system (*Pnma*) changes to two monoclinic domains below 209 K.

Results and Discussion

Figure 1 shows synchrotron radiation x-ray oscillation photographs. The photograph at 200 K clearly displays a Bragg spot splitting into two spots along the b*-direction of the prototype lattice. This split recovers to normal Bragg spots at 220 K. Therefore, the splitting of the Bragg spots indicates the existence of a structural phase transition in the temperature region 200 < T < 220 K.

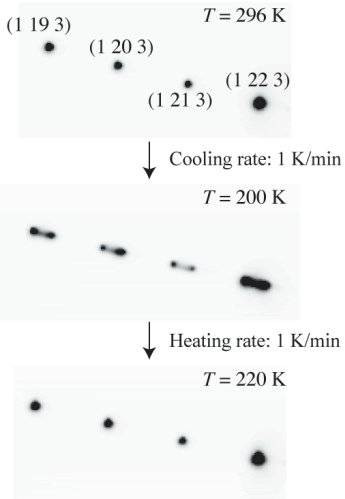

Figure 1: X-ray oscillation photographs.

In order to determine the low-temperature lattice system, x-ray diffraction measurements were carried out using a four-circle diffractometer. Figure 2 shows peak profiles of the (0 0 2) reflection. Only the (0 0 l) reflections split into two along the b*-direction of the prototype lattice below 209 K. This shows that only the interaxial angle α deviates from 90°; the b-axis tilts in the bc-plane of the prototype lattice in the real space. The low-temperature structure is composed of two monoclinic domains.

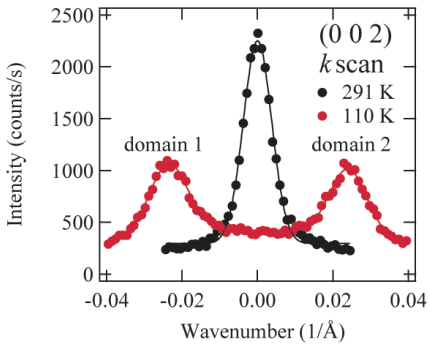

Figure 2: High- and low-temperature peak profiles.

Group-theoretical consid l ration gives us the low-temperature space group from the number of variants [2]. The low-temperature space group is $P2_1/n11$, this means that the low-temperature monoclinic phase has two crystallographically independent dimers in a conducting layer. This suggests that the present compound potentially borders on the checkerboard type charge ordered state.

References

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[2] G. Van Tendeloo et al., Acta Crystallogra. A **30**, 431 (1974).

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