The structural study of ferroelectric molecular conductor α'- $(BEDT\text{-}TTF)_2IBr_2$ by synchrotron X-ray at low temperature

Chibon Hyon[1], Masashi Watanabe[2], Kensuke Kobayashi[3], Reiji Kumai[4], Kaoru Yamamoto[5], Kyuya Yakushi[5], Yukio Noda[1]

[1]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 980-8577 Sendai, Japan

[2]Graduate school of Engineering, Tohoku University, 980-8577, Sendai, Japan

[4]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8562, Japan

[3]CMRC/PF, KEK, 305-0801, Japan [5]Institute for Molecular Science, Okazaki, Aichi 444-8585, Japan

The quasi-two dimensional molecular conductor α'-$(BEDT\text{-}TTF)_2IBr_2$ [BEDT-TTF :bis(ethylendithio)-tetrathiafulvalene] shows semi-conductive behavior at all temperature region. Recently, it was reported that this compound exhibited successive phase transitions, and the scheme of the phase transition was speculated as a charge ordering at 204 K, a ferroelectric phase transition at 160 K and a transition to non-magnetic state at 30 K [1].

The ferroelectric phase transition at 160 K seems to be different from conventional displacive type nor order-disorder type ferroelectric transitions. It is thought that electrical polarization is caused by the charge ordering of π-electrons. Such electronic origin ferroelectricity in organic conductor was not known except for α-$(BEDT\text{-}TTF)_2I_3$[2] before this compound. Furthermore, this compound exhibits three phase transitions at low temperature, in spite of the space group $P\bar{1}$ that consists of only inversion symmetry at 300 K. However, there are few structural evidences for these phase transitions.

In this report, we focus on charge ordering and ferroelectric phase transition. To reveal a relationship between these macroscopic physical properties and the microscopic crystal structures, we conducted several X-ray diffraction experiments using synchrotron radiation and conventional X-ray source. A four-circle X-ray diffractometer (HUBER Co.) at Tohoku University and an imaging plate (IP) camera at the beam line 8A in Photon Factory, KEK were used for this study. The samples were synthesized in Institute for Molecular Science. The temperature dependence of lattice parameter γ (upper) and the integral intensity of the Bragg reflection -9 -2 8 (lower) are shown in Fig. 1. Anomalies were found at 204 K and 160 K. The temperature dependence of other lattice parameters and the integral intensities of several Bragg reflections will be reported in the conference hall on the day.

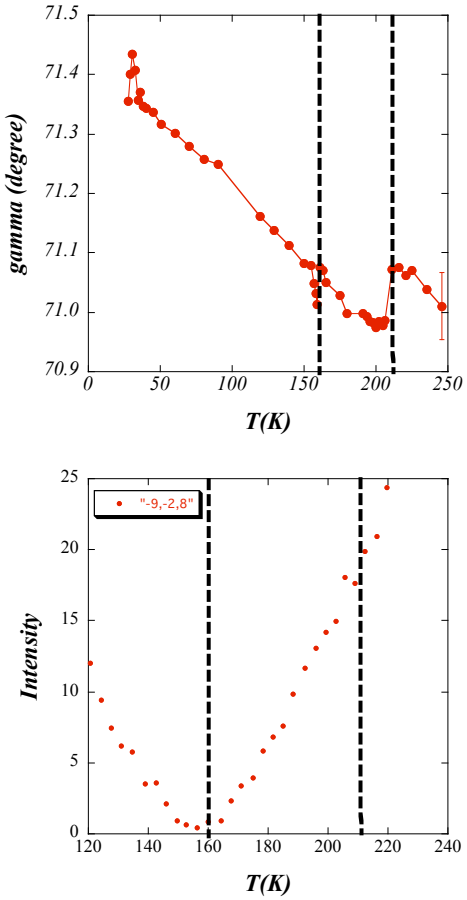

Fig.1 Temperature dependence of lattice parameter γ (upper) and integral intensity (-9 -2 8) (bottm)

[1] Y. Yue et al., JPSJ, **78**(2009), 0044701
[2] Kaoru YAMAMOTO et al., JPSJ, **77**(2008), 074709