Crystal structure and physical properties of a new organic conductor κ′′-(ET)$_2$Cu[N(CN)$_2$]Br

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The organic conductors κ-(ET)$_2$X have attracted much attention because of their striking physical properties such as superconductivity and quantum spin liquid, where ET denotes bis(ethylenedithio)-tetrathiafulvalene. They are strongly correlated electron systems and possess some similarities to high T_c cuprates such as 2D conducting layers and superconductivity in the vicinity of Mott insulating phase.

Among them, κ-(ET)$_2$Cu[N(CN)$_2$]Br (κ-Br) is an ambient-pressure superconductor with a relatively high T_c = 11.6 K in close proximity to Mott insulating state[1], whereas its derivative κ-(ET)$_2$Cu[N(CN)$_2$]Cl (κ-Cl) is an antiferromagnet and shows a Mott and a superconducting transition with T_c = 12.8 K under a mild pressure of 0.3 kbar[2]. It has been considered that the electron correlation is a key factor dominating the ground states of κ-(ET)$_2$X [3].

Recently, we found a new polymorph of κ-Br, κ″-(ET)$_2$Cu[N(CN)$_2$]Br (κ″-Br), which was obtained as a by-product of κ-Br. The κ″-Br salt has a monoclinic crystal structure composed of conducting ET layers and insulating anion layers alternating along *a* axis (Fig. 1). The molecular long axis of ET is nearly collinear in the monoclinic κ″-Br, while there are alternating two kinds of ET layers with different orientation in the orthorhombic κ-Br. The κ-type arrangement of ET molecules in κ″-Br is similar to that of κ-Br. In the polymeric zig-zag chains of anions, the dicyanamide groups are disordered in κ″-Br, while they are ordered in κ-Br.

We also report the band structure and physical properties of κ″-Br and discuss its electronic states.

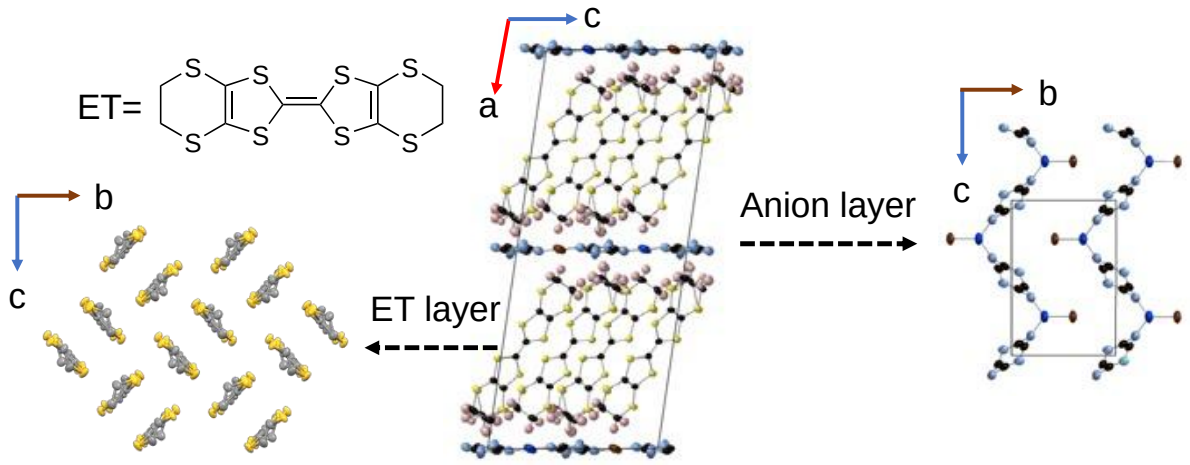

Fig. 1. Crystal structure of κ″-(ET)$_2$Cu[N(CN)$_2$]Br.

References

[1] A. M. Kini *et al.*, *1norg, Chem.* **29**, 2555-2557 (1990).
[2] Jack M. Williams *et al.*, *1norg, Chem.* **29**, 3272-3274 (1990).
[3] K. Kanoda, *J. Phys. Soc. Jpn.* **75**, 051007 (2006).