Crystal structure and physical properties of a new organic conductor κ''-$(ET)_2Cu[N(CN)_2]Br$

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The organic conductors κ-$(ET)_2X$ have attracted much attention because of their striking physical properties such as superconductivity and quantum spin liquid, where ET denotes bis(ethylenedithio)-tetrathiafulvalene.

Among them, κ-$(ET)_2Cu[N(CN)_2]Br$ (κ-Br) is an ambient-pressure superconductor with a relatively high critical temperature T_c = 11.6 K in close proximity to a Mott insulating state[1], whereas the isostructural κ-$(ET)_2Cu[N(CN)_2]Cl$ (κ-Cl) is an antiferromagnet and shows a pressure-induced superconductivity at 12.8 K under a moderate pressure of 0.3 kbar[2]. It has been considered that the electron correlation is a key factor dominating the ground states of κ-$(ET)_2X$ [3].

Recently, we found a new polymorph of κ-Br, κ''-$(ET)_2Cu[N(CN)_2]Br$ (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 orientations 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.

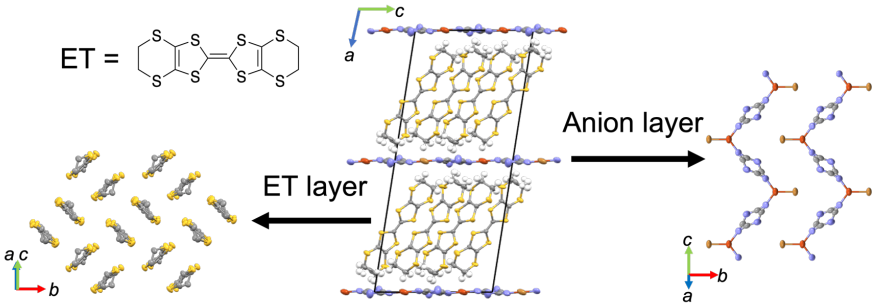

Fig. 1. Crystal structure of κ''-$(ET)_2Cu[N(CN)_2]Br$

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