

Searching for Crystallographic Superstructures in κ -(BEDT-TTF)₂Cu[N(CN)₂]Br

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Recently, we have performed a detailed investigation of the low temperature structure of the organic superconductor κ -(BEDT-TTF)₂Cu[N(CN)₂]Br [1]. Our aim was to resolve a possible structural modification of the system associated with terminal ethylene group ordering upon undergoing a glass-like transition at $T_g = 77\text{K}$ [2]. In the course of our experiments, in addition we have tested claims of a relationship between superstructure formation as result of terminal ethylene group ordering and the glass-like transition [3-5]. According to these references, half-integer peaks occur at (6 0 3.5), (7 0 3.5), (8 0 3.5) [3] and (3 0 0.5), (5 0 0.5), (7 0 0.5), (6 0 3.5) [4] at low temperatures. Here, we report on extended synchrotron x-ray diffraction experiments on two samples κ -(BEDT-TTF)₂Cu[N(CN)₂]Br carried out at the 7T multipole wiggler beamline MAGS at BESSY, HZB, in vertical scattering four-circle geometry at a photon energy of 12.398keV. To avoid irradiation damages the beam intensity was reduced using absorber foils. Surprisingly, in our low temperature (28K) experiments, when searching k -space at (6 0 3.5), (7 0 3.5), (8 0 3.5), (3 0 0.5), (5 0 0.5), (7 0 0.5) for both samples, for none of these spots we could detect scattering intensity as result of superstructure formation, in contradiction to the observations in the Refs. [3,4]. Our data suggest that details of the structural properties of κ -(BEDT-TTF)₂Cu[N(CN)₂]Br – such as superstructure formation – sensitively depend on sample handling, *e.g.*, cooling rates (in our case 4K/min), or thermal cycling. A direct relationship between superstructure formation and terminal ethylene group ordering cannot be verified, disproving the proposal put forth in Ref. [5].

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