[MS33-P05] High pressure crystal structure of the κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ superconductor
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In the pressure-temperature phase diagram of the κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ crystals, a Mott insulator (spin liquid), metal (Fermi liquid) and superconducting states converge near 3.5kbar-4K point [1]. We investigated the structure of the twinned crystal samples at room temperature and 4kbar using diamond anvil high pressure cell and at 150K at normal pressure. The pressure-temperature points above are very special ones for structure analysis, for twinning turns to be pseudomerohedry at these conditions. In this report we analyze the crystal structure transformations and modifications of the triangular spin lattice parameters due to high pressure. At a first approximation the molecular orbital overlap integrals, which are characteristics of the spin lattice, change in isotropic way. We suppose that at 4 kbar hydrostatic pressure the crystal is located near the Mott insulator – superconductor phase boundary when cooled down below 4K.


Keywords: high-pressure structure determination, organic conductors superconductors, electronic structure