

**MS15-P37** Pressure and temperature dependence of charge transfer behaviour of the  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub> organic conductor.

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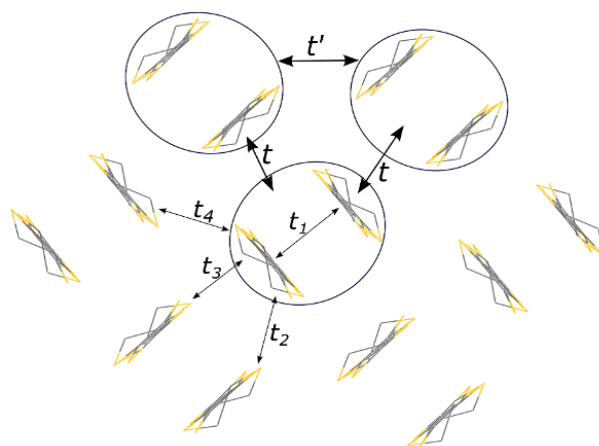
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Since 1982 when the first metallic compound based on adjusted  $\pi$ -conjugated donor BEDT-TTF (ET) molecules has been found the interest to organic complexes with quasi-2D electronic structure has been only increasing. The  $\kappa$ -type ET<sub>2</sub>X salts with polymer-like inorganic anions X=Cu<sub>2</sub>(CN)<sub>3</sub> deserved a great attention due to their superconducting properties and spin-frustration possibilities within the anisotropic triangular sublattice of the face-to-face pair of ET molecules. The origin of this superconductivity can be found in quantum spin liquid and caused by spin interaction in half-filled triangular lattice in this type Mott insulator. In the pressure-temperature phase diagram of the  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu<sub>2</sub>(CN)<sub>3</sub> 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 untwinned crystal samples at low temperatures and elevated pressures. X-ray diffraction data were collected in the 90K - 300K temperature region at ambient pressure and from ambient to 8 kbars pressure at room temperature using Oxford Diffraction Gemini-R diffractometer with Atlas CCD detector (MoK $\alpha_1$ =0.71073Å, graphite monochromator,  $\omega$ -scan method), Diacell Bragg-(S) Plus diamond anvil cell for high pressure experiments and Oxford CryoJet Systems to provide the temperature control during experiments. In this report we analyze the crystal structure transformations and modifications of the triangular spin lattice parameters due to high pressure in comparison with the temperature changes. The values of transfer integrals  $t'$  and  $t$  were calculated by site-energy correction and band-fitting methods within density functional theory. The difference between results of these two approaches is discussed.

The reported study was supported by RFBR, grant No14-02-01150

References

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**Figure 1.** Dimer of ET molecules as an unit of  $\kappa$ -type salts arrangement and transfer integrals.

**Keywords:** crystallography, high pressure, organic conductive materials