# 低温物質科学研究センター セミナー

(平成 17 年度 第 5 回)

(21 世紀 COE 京都大学化学連携研究教育拠点 共催)

# Synthesis peculiarities and properties of the radical cation salts, κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]X


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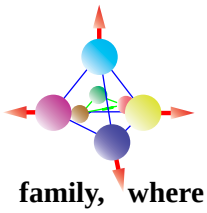
日時 ： **2005 年 10 月 7 日 (金) 16:00- [October 7]**

場所： 理学部 **6** 号館 **402** 号室 **(**理学部 6 号館南棟**)**

**Room 402 Faculty of Science Bldg. No.6**




**Abstract**

**Isostructural radical cation salts of the κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]X family, where BEDT-TTF is an organic π-donor, bis(ethylenedithio)tetrathiafulvalene, X= Br, Cl, I, Br$_{1-x}$Cl$_x$, Br$_{1-x}$I$_x$, have intensely been studied over past years . They demonstrate a wide variety of electron properties despite of their similar crystal structures. These compounds are layered materials built of conducting radical cation BEDT-TTF layers, which alternate with dielectric ones composed of {Cu[N(CN)$_2$]X}$^-$ anions . The anion sheet consists of polymeric zig-zag chains extended along the *a* direction, which involve a flat three- coordinated Cu$^+$ ion with two bridged [(NC)N(CN)] groups and a terminal halogen X atom. The radical cation layer is formed by pairs of the BEDT-TTF molecules, which are packed perpendicular to each other in a crystal. According to theoretical calculations of band structure, these materials are expected to be metals. It was found that radical cation salts with X =Br, Br$_{0.5}$Cl$_{0.5}$ and Br$_{0.7}$Cl$_{0.3}$ are ambient pressure organic superconductors with *Tc* = 11.6 K, while salts with X = Cl and Br$_{0.9}$I$_{0.1}$ undergo a superconducting transition at 0.3 kbar with *Tc* = 12.8 K and 3.5 K , respectively , and a salt with X = I exhibits a superconducting transition at 1.2 kbar with *Tc* ≈ 8 K.**

**Recently we prepared single crystals of the new κ'-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl salt (κ'-Cl), which in contrast to the described Mott insulator, κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, have metallic properties and undergo a superconducting transition with *Tc* =11.5 K at ambient pressure. X-ray analysis of these crystals was performed and physical properties were studied. The crystals of κ'-Cl show some distinctions in structure as compared to that of the κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl: smaller size of the unit cell ("chemical compression"), deficiency (5%) of the occupancy of copper positions and another ratio of eclipsed and staggered conformations in crystals (0.8:0.2 at room temperature).**

**The conformational states of the BEDT-TTFs, determined by different (eclipsed and staggered) orientation of the terminal ethylene groups, are disorder at room temperature, and tend towards eclipsed order on cooling. The salts of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]X family show a complicated sequence of structural transformations, which depend on the synthesis conditions. Structural transformations in κ-(BEDT-TTF)$_2$[CuN(CN)$_2$]I were studied by the use of diffraction x-ray analysis. It was found that in the highest quality crystals the glass transformation can be resolved into at least two superstructures with different modulation periods. The main features of the phase diagram of the glass transformation of these salts can be reasonably understood in an axial next-nearest-neighbour-interaction type model.**



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