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Mott transition in the organic compound κ -(BEDT-TTF)₂ Cu[N(CN)₂]Cl: An evidence for two energy scales

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Abstract. We have performed in-plane transport measurements on the two-dimensional organic salt κ -(BEDT-TTF)₂ Cu[N(CN)₂]Cl. A variable gas pressure technique allows for a detailed study of the changes in conductivity through the insulator-to-metal transition. We identify four different transport regimes as a function of pressure and temperature corresponding to insulating, semi-conducting, "bad metal", and strongly correlated Fermi liquid behaviours.

Key words. Mott transition – strongly correlated material – organic salt – high pressure.

1. MOTT TRANSITION IN THE ORGANIC COMPOUND κ -(BEDT-TTF)₂ Cu[N(CN)₂]Cl

The Mott metal-insulator transition (MIT) is a key phenomenon in the physics of strongly correlated electron materials (for a review, see Ref. [1]). This issue is particularly important in view of recent theoretical predictions [2] which should be put to experimental test. Layered charge-transfer salts of the κ -(BEDT-TTF)₂ X family (where X is a monoanion) offer a remarkable opportunity for such a study. The κ -(BEDT-TTF)₂ Cu[N(CN)₂]Cl compound in particular (abbreviated κ -Cl below) displays a very rich phase diagram with paramagnetic insulating, antiferromagnetic insulating, superconducting and metallic phases when pressure is varied over a range of a few hundred bars [3-5].

In this work, we report on an extensive experimental study of the in-plane resistivity of the κ -Cl compound for a range of pressure spanning both the insulating and the metallic phases, between 1 bar and 1 kilobar. In contrast to previous studies, pressure is varied continuously using a Helium gas cell, at constant temperature from 13 up to 52 K. By analyzing the pressure and temperature dependence of the measured resistivity, we have identified important crossover lines, which are summarized on the phase diagram of Fig.1.a. These crossovers separate four different regimes of transport within the paramagnetic phase, corresponding to an "insulator", a "semiconductor", a "bad metal" and a Fermi-liquid metallic regime.

The data clearly demonstrate how pressure drives the system from a low-conductivity insulating regime at low pressure (below 200 bar) to a high-conductivity metallic regime at high pressure (above 350 bar), with a more complex transition region in the 200-350 bar range [6]. Our measurements were performed both with increasing and decreasing pressure sweeps, yielding a determination of the two spinodal lines $P_{C1}^C(T)$ and $P_{C2}^C(T)$ shown in Fig. 1.a.

The pressure interval in which the normalized difference of conductivity between these two measurements exceeds our experimental precision [6] corresponds to the region of coexistence between in the insulating and metallic phases. This interval is found to be rather large (≈ 100 bar) at 35 K, and still measurable at 39 K. Our measurements yield a determination of the critical point in the $T_C \approx 39$ K to $T_C \approx 42$ K range ($P_C \approx 280$ bar).

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Figure 1. a : Pressure-Temperature phase diagram of the κ -Cl salt. The crossover lines identified from our transport measurements delimit four regions, as described in the text. The spinodal lines define the region of coexistence of insulating and metallic phases (hatched). The transition line into an antiferromagnetic insulating phase has been taken from Ref. [5], while the superconducting phase [4,5] below 13 K has been omitted. **b :** Pressure-dependence of the Mott gap, metallic crossover T^* and quasi-particle energy ε_F^* . It's worthy to note the accordance between T^* and ε_F^* .

2. AN EVIDENCE FOR TWO ENERGY SCALES

At low temperature (below 50 K), an activation law $\rho = \rho_0 \exp(\Delta(P)/2T)$ describes the data quite well in the Mott insulating regime, while a crossover to a different insulating regime [6] is observed at higher temperatures (Fig.1.a). An approximately linear pressure dependence of $\Delta(P)$ Fig.1.b is found. Hence, the activation gap is still a *large scale* close to the coexistence region, and a rough extrapolation would lead to a gap closure around 370 bar, suggesting that the finite-temperature Mott transition is *not driven* by the closure of the Mott gap.

In the metallic side, the resistivity has a quadratic Fermi liquid dependence upon temperature: $\rho = \rho_0 + A(P)T^2$, up to the coherence temperature T^* defining the onset of a “bad metal” regime (Fig.1.a). The prefactor $A(P)$ is found to depend strongly on pressure, and the product $A(P)T^{*2}$ remains approximately pressure-independent. These findings correspond to a strongly correlated Fermi liquid regime at low temperature with a renormalized Fermi energy ε_F^* . The data suggest a divergency of A and a vanishing of ε_F^* , with $A \approx (\hbar/e^2)d/\varepsilon_F^{*2}$, at P of order 150 bar, significantly smaller than the pressure at which the extrapolated insulating gap would vanish (Fig.1.b). This suggests that the closure of the Mott gap and the loss of Fermi liquid coherence are two distinct phenomena, associated with very different energy scales, as is also clear from the fact that the coherence scale T^* or ε_F^* is much smaller than the insulating gap Δ . Finally, we observe that our data *in the critical regime* around (T_C, P_C) do not appear to obey the critical behaviour observed in the doped vanadium oxide compound [7].

To conclude, we have performed detailed transport measurements on the κ -Cl compound using a variable pressure technique. Four transport regimes have been identified as a function of temperature and pressure, separated by crossover lines. Both metallic and insulating transport properties suggest a separation of energy scales in accordance with DMFT scenario.

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