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α And β-(BEDT-TTF)$_2$ $^{+}I^{-}$ $_3$: Two Dimensional Organic Metals

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α- AND β-(BEDT-TTF)$_2^+I_3^-$: TWO DIMENSIONAL ORGANIC METALS

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Abstract Electronic properties of α- and ß-(BEDT-TTF)$_2$I$_3$ crystals are reported.

BEDT-TTF [bis(ethylendithio)tetrathiofulvalene] salts have caused considerable interest, since Saito et al.[1] have proved strong intermolecular contacts and exchanges in more than one direction. Additionally, Parking et al.[2] reported a superconducting transition in a ReO_4^--derivative under pressure. Electrochemical methods using I_3^- as counterions yield several crystallographic phases[3-7], with different physical properties, e.g. α-(BEDT-TTF)$_2^+I_3^-$ (α-1) and ß-(BEDT-TTF)$_2^+I_3^-$ (ß-1). The former has a metal to insulator transition at 135 K[3-4] which can be supressed above 15 Kbar[8]. ß-1 stays metallic down to 1.4 K. There the crystals become superconducting at ambient pressure[5,8]. Other triiodide phases seem to show superconducting transitions even at 2.5 K[6,7]. Figure 1 shows the projection of the unit cells of α-1 onto the bc-plane (left) and of ß-1 onto the ac-plane. Both phases crystallize in the triclinic space group $P\bar{1}$ (α-1: a = 9.211 Å, b = 10.850 Å, c = 17.488 Å, α = 96.95°, ß = 97.97°, γ = 90.75°; ß-1: a = 6.615 Å, b = 9.097 Å, c = 15.291 Å, α = 94.35°, ß = 95.55°, γ = 109.75°)

and are two dimensional organic metals.

The first order phase transition in α-1 at 135 K can be utilized to demonstrate the validity of the Wiedemann-Franz-law $K_e/\sigma = \pi^2/2 \cdot k_B^2/e^2 \cdot T = L_o \cdot T$. Here K_e is the thermal conductivity of

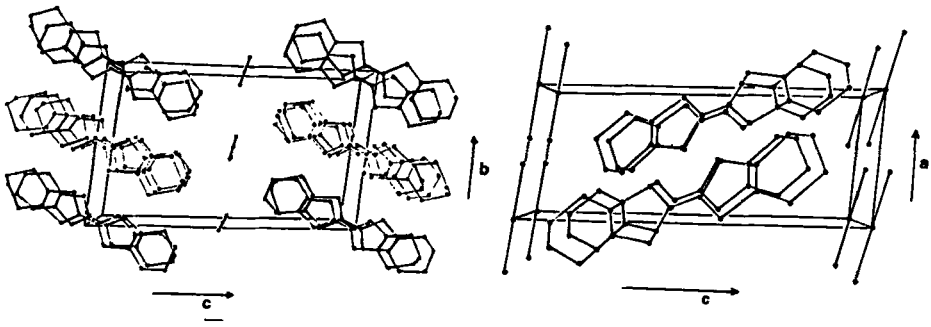

Fig. 1) Structure of α-1 (left) and ß-1 (right).

the charge carrier, σ the electrical conductivity, T the temperature and $L_o = 2.44 \cdot 10^{-8} V^2/K^2$ the Lorentz-number. Fig. 2 shows the temperature dependence of the total thermal conductivity K shows the tals of α-1. Assuming that the difference of 1.5 mW/(cm·K) in K at 135 K is due to the contribution K_e of the charge carriers in the metallic range and taking the typical value of the electrical conductivity at 135 K $\sigma_{135} = 450(\Omega\,cm)^{-1}$ we obtain a value

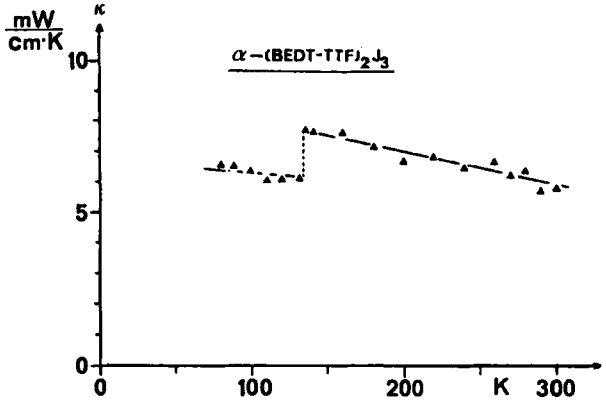

Fig. 2) Thermal conductivity of α-1.

$K_e/(\sigma_{135} \cdot T) = 2.5 \cdot 10^{-8} V^2/K^2$. Even if we assume that σ_{135} is only correct within an error of 20 % this value agrees quite well with the Lorentz-number. In addition the results of Fig. 2 demonstrate that in an organic metal the contribution to K due to the lattice phonons predominates the contribution of the charge carriers in contrast to the usual metals.

In our preparation of α-1 using THF[3,4] we always observed canted rhombohedrons of ß-1. Fig. 3 shows the microwave conductivity as measured at 10 GHz by the cavity perturbation method between 3 and 300 K. A very similar temperature dependent conductivity behaviour was observed with dc-methods. Typical room temperature conductivities range around $35(\Omega\,cm)^{-1}$. Nevertheless, the peak in the microwave conductivity at about 125 K is sensitive to the microwave power. For somewhat higher microwave field strength (x) the conductivity increases stronger and already at higher temperatures ($T \simeq$ 200 K). Further experiments are in progress in order to explain this behaviour.

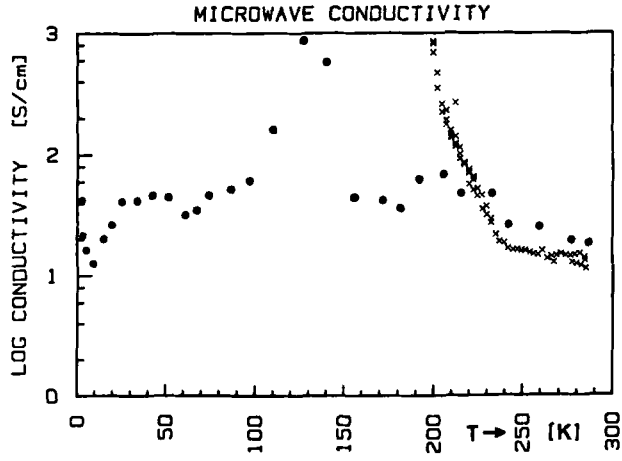

Fig. 3) Microwave conductivity at 10 GHz of ß-1.

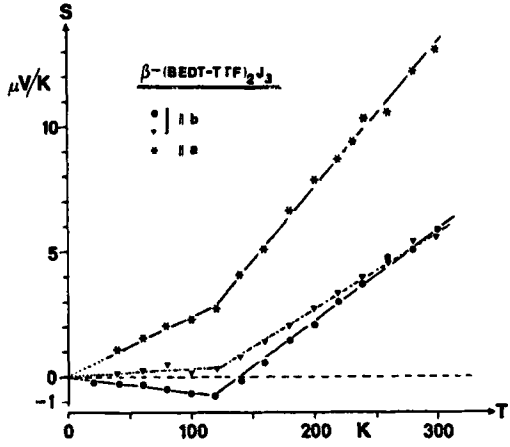

Fig. 4)
Thermopower of ß-1.

ESR-experiments indicate a temperature independent susceptibility between 300 and 4.2 K. The ESR-linewidth at room temperature can be used to discriminate between α-1 and ß-1 (70 to 110 Gauss for α-1 and 20 to 25 Gauss for ß-1 depending on the orientation of the crystals with respect to the magnetic field).

Temperature dependent thermopower measurements prove a metallic state down to low temperatures (Fig. 4) but around 120 K a phase transition might occur. From the slope of the thermopower above 150 K it can be estimated that the width of the conducting band in a-direction is about 2/3 of the bandwidth in b-direction in good agreement with optical reflectance measurements[10]. Volume superconductivity in ß-1 at ambient pressure and a diamagnetic transition temperature of 1 K is reported separately[8].

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