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OPTICAL INVESTIGATIONS OF THE ELECTRICAL ANISOTROPY OF α- AND β- $(BEDT\text{-}TTF)_2I_3$ *

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Abstract The anisotropy of the electrical transport properties at room temperature of the α- and β-phase of $(BEDT\text{-}TTF)_2I_3$ was determined from the polarized reflectance spectra.

INTRODUCTION

Among the BEDT-TTF radical salts the $(BEDT\text{-}TTF)_2I_3$ has now attracted special interest, because superconductivity at ambient pressure has been recently observed in the β-phase of this compound[1]. Like the other metallic salts of this family,both $(BEDT\text{-}TTF)_2I_3$ phases show metallic conduction in two dimensions. It was the aim of the present paper to determine the principal axes of the tensor of the electrical conductivity, of the effective mass, and of the collision time of the free carriers, and further to estimate the values of the band width and of the mean free path.

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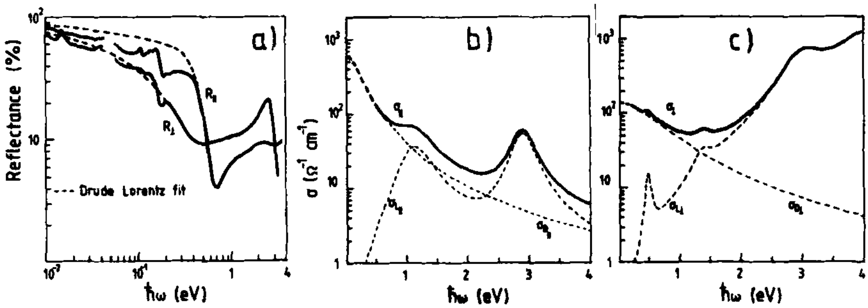

FIGURE 1 Polarized reflectance spectra (a) and conductivity functions $\sigma_{\parallel}$ (b) and $\sigma_{\perp}$ (c) of α-(BEDT-TTF)$_2$I$_3$, (001) plane

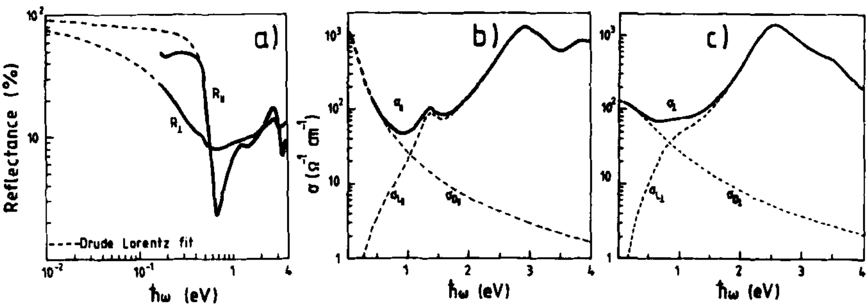

FIGURE 2 Polarized reflectance spectra (a) and conductivity functions $\sigma_{\parallel}$ (b) and $\sigma_{\perp}$ (c) of β-(BEDT-TTF)$_2$I$_3$, (001) plane.

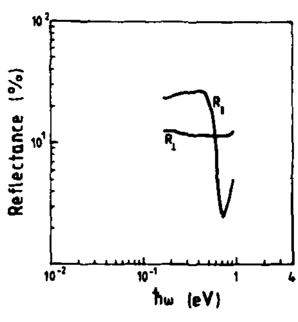

FIGURE 3 Polarized reflectance spectra of β-(BEDT-TTF)$_2$I$_3$, (100) plane.

CRYSTALLOGRAPHIC AND EXPERIMENTAL DETAILS

Both phases crystallize in the triclinic space group P1 (α-phase: a = 9.211 Å, b = 10.850 Å, c = 17.488 Å, α = 96.95°, β = 97.97°, γ = 90.75°, Z = 2; β-phase: a = 6.615 Å, b = 9.097 Å, C = 15.291 Å, α = 94.35°, β = 95.55°, γ = 109.75°, Z = 1)[2-4] and show metallic conduction parallel to the (001) plane. This plane includes the stack axis of the BEDT-TTF molecules, which is in the α-phase parallel to the [100] and in the β-phase parallel to the [110] direction. The reflectance spectra were generally obtained on (001) surfaces with the exception of Fig.3, where a (100) surface of the β-phase was investigated.

EXPERIMENTAL RESULTS AND DISCUSSION

Fig.1 to 3 show the polarized reflectance spectra of both phases at room temperature. In Fig.1 and 2 the directions of polarization coincide with the principal axes of the tensor of the optical conductivity. This was found by stepwise rotation of the polarizer. The existence of plasma edges of different shape and different spectral position for the two directions of polarization indicates a remarkable anisotropy of the electrical properties within the metallic plane for both phases. Analyzing $R_{\parallel}$ and $R_{\perp}$ by a Lorentz-Drude model, the spectral distribution of the conductivity functions are obtained. These functions can be extrapolated to zero energy leading to an optical value for the dc-conductivity. It is interesting to note that in the α-phase the direction of the highest metallic conductivity $\sigma_{0\parallel}$ is found to be nearly perpendicular to the stack axis. That means that in this case the orbitals of the BEDT-TTF molecules overlap preferably side by side and not along the stack axis.

On the contrary in the β-phase the highest conductivity extends along the stack axis. In Fig.3 the nearly constant reflectance spectrum $R_\perp$ which belongs to the direction of polarization perpendicular to the metallic plane, shows the lack of metallic conduction along the c-axis.

As the free carrier concentration N is known from the chemical composition, also the principal axis of the effective mass tensor m^* can be calculated from the optical results. On the basis of the tight-binding model further the band width 4t in the direction of the principal axes of the conductivity tensor, the Fermi velocity V_F, and the mean free path Λ can be estimated.

TABLE I Transport properties of $(BEDT\text{-}TTF)_2I_3$

		N ($10^{21}/cm^3$)	m^*/m_o	τ (10^{-15}s)	4t (eV)	V_F (10^{15}Å/s)	Λ (Å)
α	[010]	1.16	1.3	2.5	1	2.8	7
	[100]		3.2	1.3	0.4	1.8	2.3
β	[110]	1.16	1.3	4.2	0.9	2.9	12
	[1$\bar{3}$0]		2.2	0.9	0.6	2.2	2

REFERENCES

1. E.B.Yagubskii, I.F.Schegolev, V.N.Laukhin, P.A.Kononovich, M.V.Kartsovnic, A.V.Zvarykina, and L.I.Buravov, Pis'ma Zh.Eksp.Teor.Fiz. 39, 12 (1984).
2. K.Dietz, H.Endres, H.W.Helberg, J.Henning, H.J.Keller H.W.Schäfer and D.Schweitzer, Mol.Cryst.Liq.Cryst., 107, 45(1984)
3. T.Mori, A.Kobayashi, Y.Sasaki,H.Kobayashi,G.Saito and H.Inokuchi, to appear in Chem.Lett.
4. J.Henning, K.Bender, D.Schweitzer, U.Dietz, H.Endres, and H.J.Keller, Proceedings: Physics and Chemistry of Low-Dimensional Synthetic Metals, Abano Terme, Mol. Cryst.Liq.Cryst., in print.