Abstract Submitted
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Organic Conductors

Electronic Structure of $(TMTSF)_2PF_6$. P.M. GRANT, IBM San Jose--The four nearest neighbor dimer splittings of TMTSF in $(TMTSF)_2PF_6$ have been calculated in the Extended Huckel Approximation. The crystal structure employed was the room temperature results of Jacobsen et al.[1] Two of the dimers considered form along the stacking direction between the two TMTSF molecules per unit cell and the other pair were chosen in the interstack direction of shortest Se-Se contact. Each dimer splitting is proportional to an appropriate transfer integral.[2] Of particular interest are the ratios of the interchain-to-intrachain dimer splittings as these scale both the normal and superconducting transport anisotropy in this material. We obtained values $22 < t_{||}/t_{\perp} < 150$ for the various dimer combinations. These results will be related to experimental findings on optical properties, normal conductivity and critical field behavior. A simple two-dimensional band structure will be presented.

1. C. Jacobsen et al., to be published in Chimica Scripta.
2. J. M. Rohr, private communication.

(X) Prefer Standard Session

P.M. Grant
Signature of APS Member

P. M. Grant
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sion between the electrons. Under suitable conditions, the model calculations indicate that the electron-electron interaction via demons can be attractive, but the results also suggest that this mechanism is probably not dominant in transition metals and transition metal compounds. An attractive interband contribution is found, and it is proposed that this effect may lead to pairing in suitable systems.
*Present address: Dept. of Physics, MIT.

SESSION AK: ORGANIC CONDUCTORS I

Monday morning, 16 March 1981
Civic Center, Room S6 at 9:00 A.M.
P. M. Chaikin, presiding

AK 1 Electronic Structure of $(TMTSF)_2PF_6$. P.M. GRANT, IBM San Jose--The four nearest neighbor dimer splittings of TMTSF in $(TMTSF)_2PF_6$ have been calculated in the Extended Huckel Approximation. The crystal structure employed was the room temperature results of Jacobsen et al.[1] Two of the dimers considered form along the stacking direction between the two TMTSF molecules per unit cell and the other pair were chosen in the interstack direction of shortest Se-Se contact. Each dimer splitting is proportional to an appropriate transfer integral.[2] Of particular interest are the ratios of the interchain-to-intrachain dimer splittings as these scale both the normal and superconducting transport anisotropy in this material. We obtained values $22<t_{||}/t_{\perp}<150$ for the various dimer combinations. These results will be related to experimental findings on optical properties, normal conductivity and critical field behavior. A simple two-dimensional band structure will be presented.

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2. J. M. Rohr, private communication.

AK 2 Shubnikov-de Haas Oscillations in $(TMTSF)_2PF_6$.* J.F. KWAK and J.E. SCHIRBER, Sandia National Laboratories Albuquerque,** R.L. GREENE and E.M. ENGLER, I.B.M., San Jose.--We report the observation of Shubnikov-de Haas-like oscillations in the resistivity of $(TMTSF)_2PF_6$ under pressure. There are, however, a number of unusual anomalies in the effect observed as compared to traditional Shubnikov-de Haas oscillations. The bulk of the data were taken by modulating the magnetic field at 50 Hz and measuring the sample voltage, with DC current input, at the 3rd harmonic of the modulation frequency. The sample was mounted in a helium pressure bomb, with the results reported here being obtained at 7.5 and 8 kbar. A maximum of five peaks periodic in reciprocal magnetic field appeared in the range 70-100 kOe, yielding a single frequency with the low value of $7.5 \pm .3 \times 10^5$G, $m^* \cong 1$ and a Dingle temperature of ~3°K. The effect appears only when the field is oriented roughly along the crystal c-axis, implying a Fermi surface consisting of thin tubes oriented along this direction.
*Supported by the U.S. Department of Energy (DOE) under contract DE-AC04-76-DP00789 and in part by the ONR.
**A U.S. DOE facility.

AK 3 Magnetoresistance and Hall Effect in $(TMTSF)_2PF_6$* P. HAEN, E.M. ENGLER and R.L. GREENE, IBM San Jose, and P.M. CHAIKIN,** UCLA--The transverse magnetoresistance of $(TMTSF)_2PF_6$ has been measured as a function of temperature, pressure and magnetic field direction. Below the metal-insulation transition (T_{MI}~12.5K at ambient pressure) $\Delta\rho/\rho$ is anomalously large and has considerable anisotropy. For example, at 4.2K and 50kOe we find $\Delta\rho/\rho$ ~10, 0.5 for H parallel to the c,b axis, respectively. The longitudinal resistance and the T_{MI} are unaffected by magnetic fields up to 80kOe. An exponentially increasing Hall effect is observed below T_{MI} for H parallel to b. Using a one-band model we estimate a lower limit for the a axis Hall mobility of $\mu \approx 10^4 cm^2/V\text{-}sec$ at 4.2K. The variation of the transverse magnetoresistance and Hall effect with electric field along the a axis has also been studied. Our Results will be related to current models for the origin of the non-linear resistivity and the metal insulator phase transition.
*Support partially by the ONR.
**Supported partially by NSF # DMR 79-08560.

AK 4 ESR and Conductivity Study of $(TMTSF)_2PF_6$* M. HARDIMAN, G. GRUNER, Univ. of CA. Los Angeles and R.L.GREENE, IBM, San Jose--$(TMTSF)_2PF_6$ undergoes a metal-to-semiconductor transition at low temperatures. The semiconducting phase is characterized by strongly nonlinear transport and unusual magnetic properties.[1,2] We have performed joint ESR and resistivity measurements to clarify the nature of the transition and to search for field induced ESR signal. The ESR signal disappears at temperature where the derivative of the resistivity has a maximum demonstrating that there is only one transition. Our initial attempts to detect dc electric field induced ESR signal were unsuccessful. Predictions based on various models, and the experimental difficulties to observe this effect will be discussed.
*Supported by NSF Grant #DMR78-27129
1W.M. Walsh, Jr, F. Wudl, G.A. Thomas, P. Nalewajek, J.J. Hauser, P.A. Lee and T. Poehler, Phys. Rev. Lett. 45, 829 (1980).
2P.M. Chaikin, G. Gruner, E.M. Engler and R.L. Greene, Phys. Rev. Lett. 8 Dec. (1980).

AK 5 Microwave Conductivity of the Solid Solutions $[(TMTSF)_{1-x}(TMDTF)_x]_2PF_6$. T. O. POEHLER, Johns Hopkins U.,* F. WUDL, Bell Labs, and D. NALEWAJEK, Allied Chemical--Solid solutions between the organic metal $(TMTSF)_2PF_6$ and the semiconductor $(TMDTF)_2PF_6$ yield a series of homogenous single crystals that display a metal-semiconductor transition in the vicinity of x = 0.5. The temperature dependence of the microwave conductivity of this series of solids has been investigated. The effect of composition on the metal-insulator transition temperature was examined with particular attention to the composition range $0 \leq x \leq 0.05$. The sensitivity of microwave conductivity to microwave power was also investigated in this range.

*Supported by NSF Grant DMR80-15318 and US Navy.

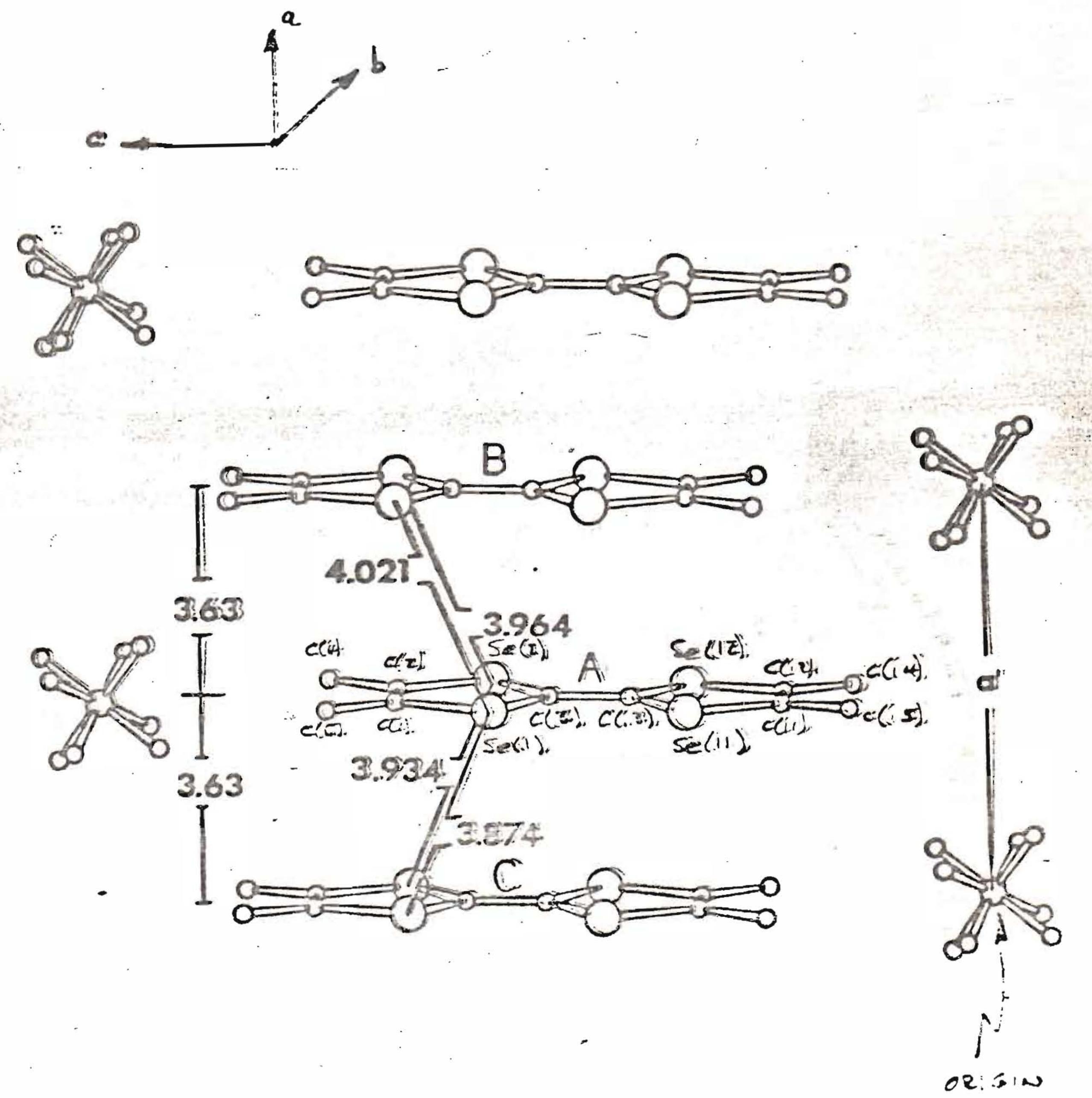
AK 6 Weak Impurity Influence on Spin Resurrection in $(TMTSF)_2AsF_6$. W. M. WALSH, JR., F. WUDL, L. W. RUPP, JR. and E. AHARON-SHALOM, Bell Labs., Murray Hill, NJ--The influence of small concentrations of tetramethyldiselenadiathiofulvalene substituted into the donor stacks of the organic metal $(TMTSF)_2AsF_6$ has been studied via magnetic resonance of the itinerant holes. Such doping produces small percentage increases in linewidth over the temperature range 300-12 K implying only a modest effect on transport scattering. The temperature of the metal-semiconductor transition remains very close to $T_{MS} \sim$ 11.5 K up to nominal concentrations of 0.2%. The principal effect of doping is found on the nonlinear recovery of spin resonance[1] below T_{MS} where the minimum spin resonance linewidth increases from 3 G in pure material to 11 G at 0.2% doping. In addition distinct stages in the spin resurrection phenomenon seen in pure material give way to a smooth recovery at the higher doping levels.

1. W. M. Walsh, Jr., F. Wudl, G. A. Thomas, D. Nalewajek, J. J. Hauser and P. A. Lee, Phys. Rev. Lett. 45, 829 (1980).

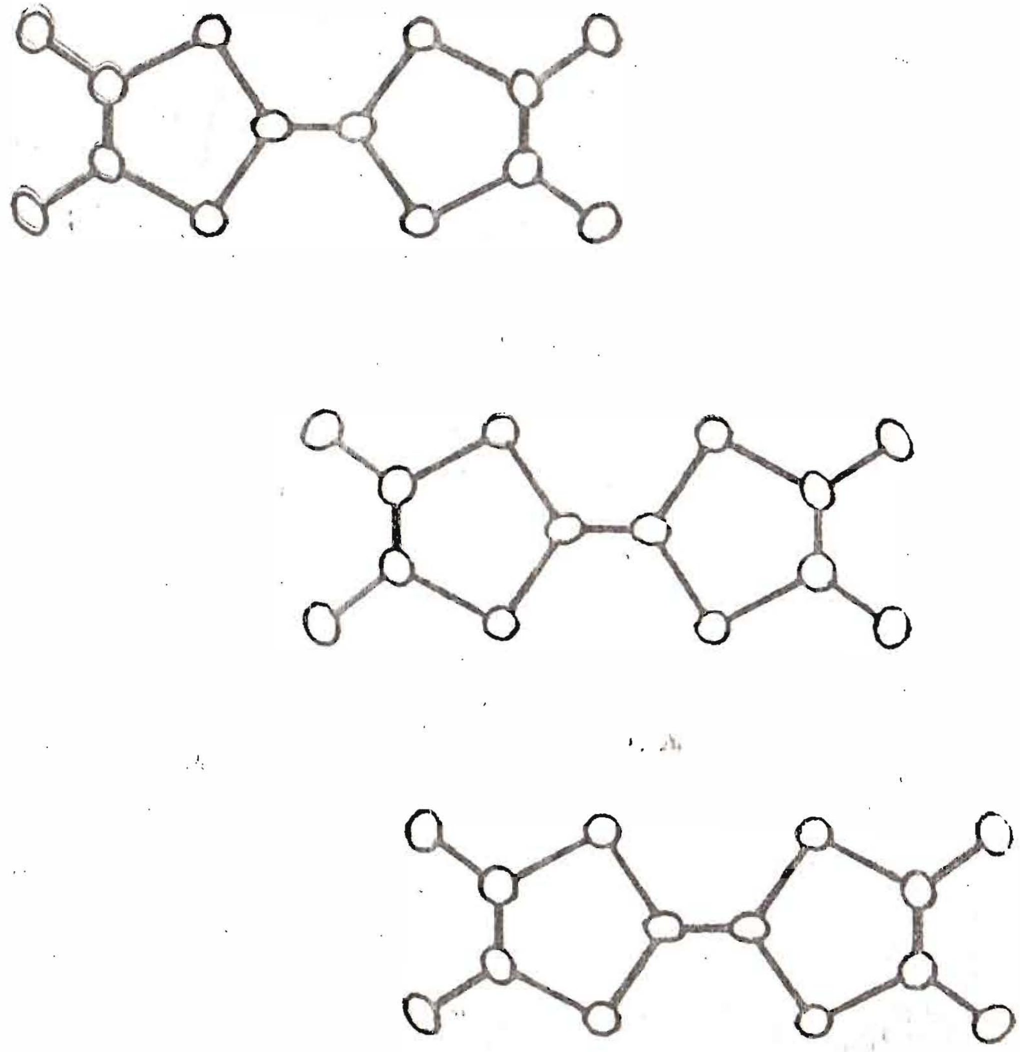
AK 7 Observation of the Meissner Effect in an Organic Superconductor. K. ANDRES*, F. WUDL, D. B. McWHAN, G. A. THOMAS, D. NALEWAJEK+, and A. L. STEVENS, Bell Labs., Murray Hill--We observe a partial Meissner effect (up to 50% at H = 0.115 Oe), fully diamagnetic shielding signals and large anisotropies in the upper critical field $[H_{c2}(||)/H_{c2}(\perp) \sim 7$ Oe/1 kOe$]$ and the lower critical field $[H_{c1}(||)/H_{c1}(\perp) \sim 0.5$ Oe/5 Oe$]$ in di- tetramethyltetraselenafulvalene-hexafluorophosphate, $(TMTSF)_2PF_6$, under applied hydrostatic pressure. We find a strong linear

PROLOGUE

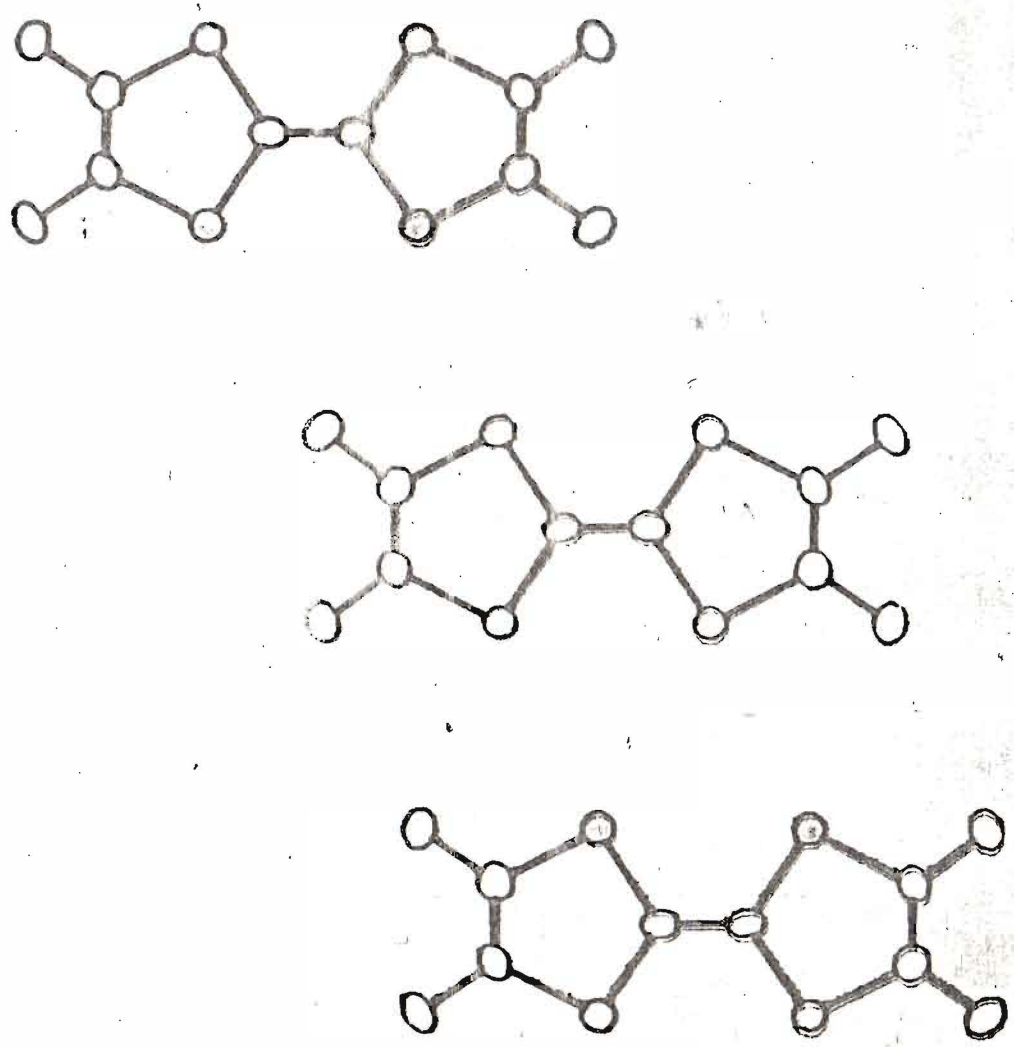
- $(TMTSF)_2 PF_6$: $T_c \sim 1°K$, $P = 6$ kbar
- $(TMTSF)_2 ClO_4$: $T_c \sim 1°K$, $P = 1$ atm
- Dependence of critical pressure on triclinic c-axis


a
b
c
B
4.021
3.63
3.964
A
3.934
3.63
3.874
C
ORIGIN

PF_6



C2O4

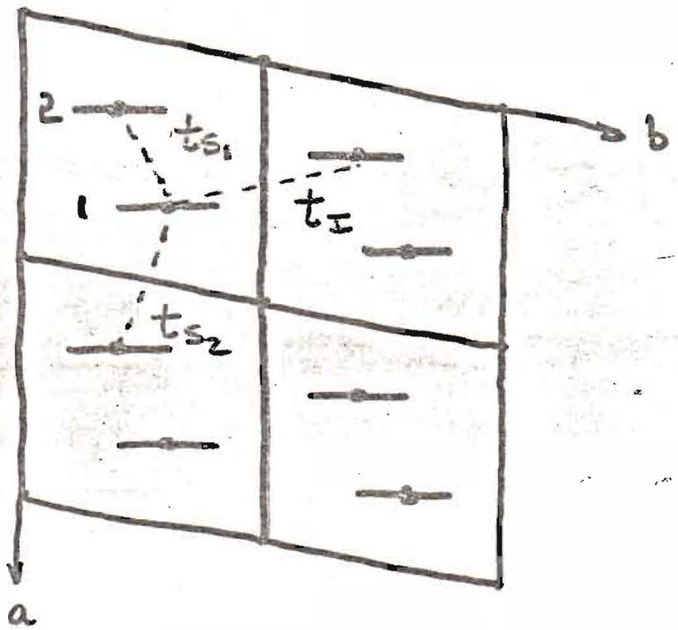


C_2O_4

PF_6

C20+

TIGHT-BINDING APPROXIMATION



$$E(k) = 2t_I \cos \vec{k}\cdot\vec{b} \pm \left\{ t_{s_1}^2 + t_{s_2}^2 + 2t_{s_1}t_{s_2} \cos \vec{k}\cdot\vec{a} \right\}^{1/2}$$

CALCULATIONAL DETAILS

→ MULLIKEN - WOLFSBERG - HELMHOLTZ - CUSACHS

$$H_{ij} = (2 - |S_{ij}|)\, S_{ij} \left\{ \frac{E_i + E_j}{2} \right\}$$

(EXTENDED HÜCKEL METHOD)

→ SLATER ORBITAL REPRESENTATION

→ NEGLECT Se 4d ORBITALS

→ $t_{ij}^{\alpha} = 0.75\, E^{\alpha} S_{ij}^{\alpha}$

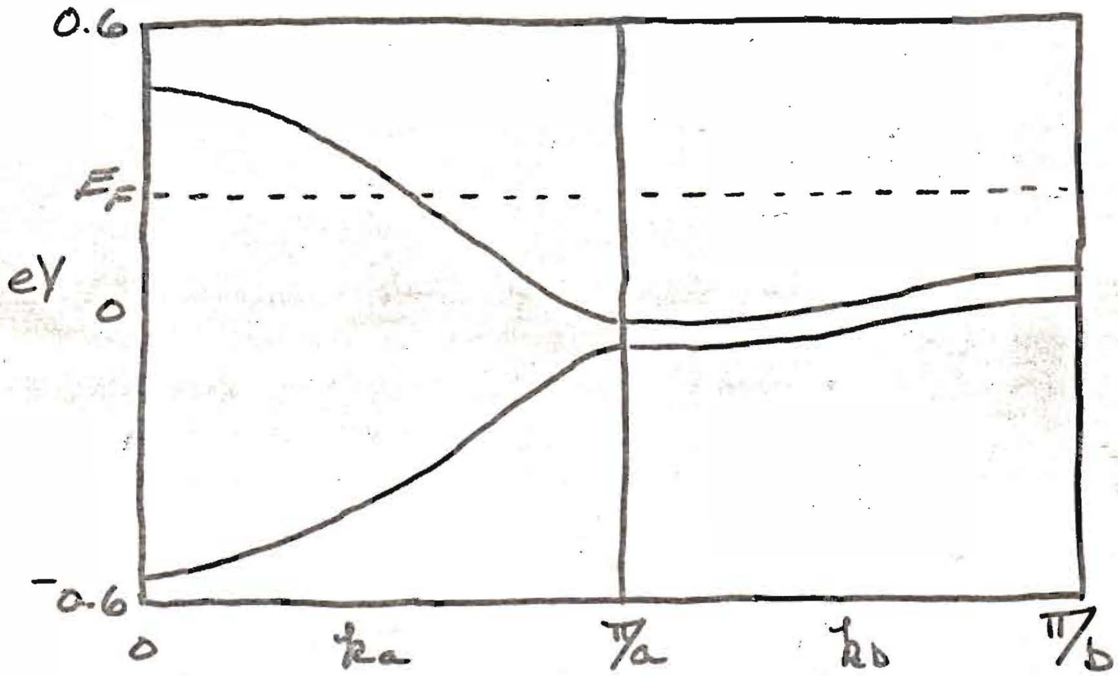
→ ALSO CHECKED BY CALCULATING DIMER SPLITTINGS WHICH SCALE AS t_{ij}

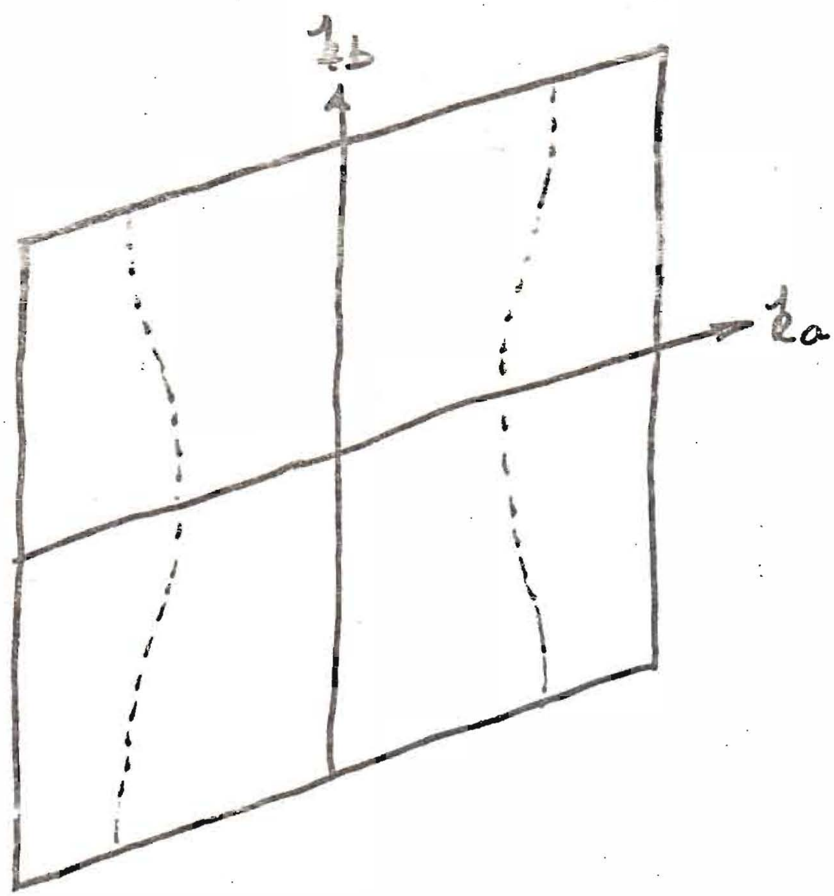
→ ANIONS PLAY PASSIVE ROLE

TRANSFER INTEGRALS & ANISOTROPY

	t_{s1}	t_{s2}	t_I	$\|A\|$
PF_6	0.28 eV	0.24	$^-$0.012	22
ClO_4	0.27	0.24	$^-$0.020	13

BAND STRUCTURE & FERMI SURFACE OF $(TMTSF)_2 ClO_4$





CONCLUSIONS

- LARGE 2D INTERACTION, ESPECIALLY WITH REGARD TO kT, BUT FERMI SURFACE DOES NOT CLOSE

- EXISTENCE OF STABLE LOW T METALLIC STATE (AND SUPERCONDUCTIVITY) DUE TO ALREADY LOW SYMMETRY AND 2:1 STOICHIOMETRY

- 2D COUPLING VERY SENSITIVE TO MINUTE SHIFTS IN INTERCHAIN POSITIONS OF TMTSF RESULTING IN OBSERVED c-AXIS DEPENDENCE OF CRITICAL PRESSURE.