

ABSTRACT SUBMITTED
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Organic Conductors

Band Structure Parameters of BEDT-TTF Charge Transfer Salts. P. M. GRANT, IBM Research Laboratories, San Jose-- We have estimated the important transfer integrals for several (BEDT-TTF) compounds from dimer splittings computed in the Mulliken-Wolfsberg-Helmholtz approximation. For the 2:1 salt containing ReO_4 , which is superconducting, we find an average anisotropy $t_{\parallel}/t_{\perp} \approx 5$, with $\langle t_{\parallel} \rangle \approx 250$ meV. Thus this compound has the lowest anisotropy of any known superconducting charge transfer salt, a result of the optimization of a key interchain interaction predicted earlier for the 2:1 salts of TMTSF.¹

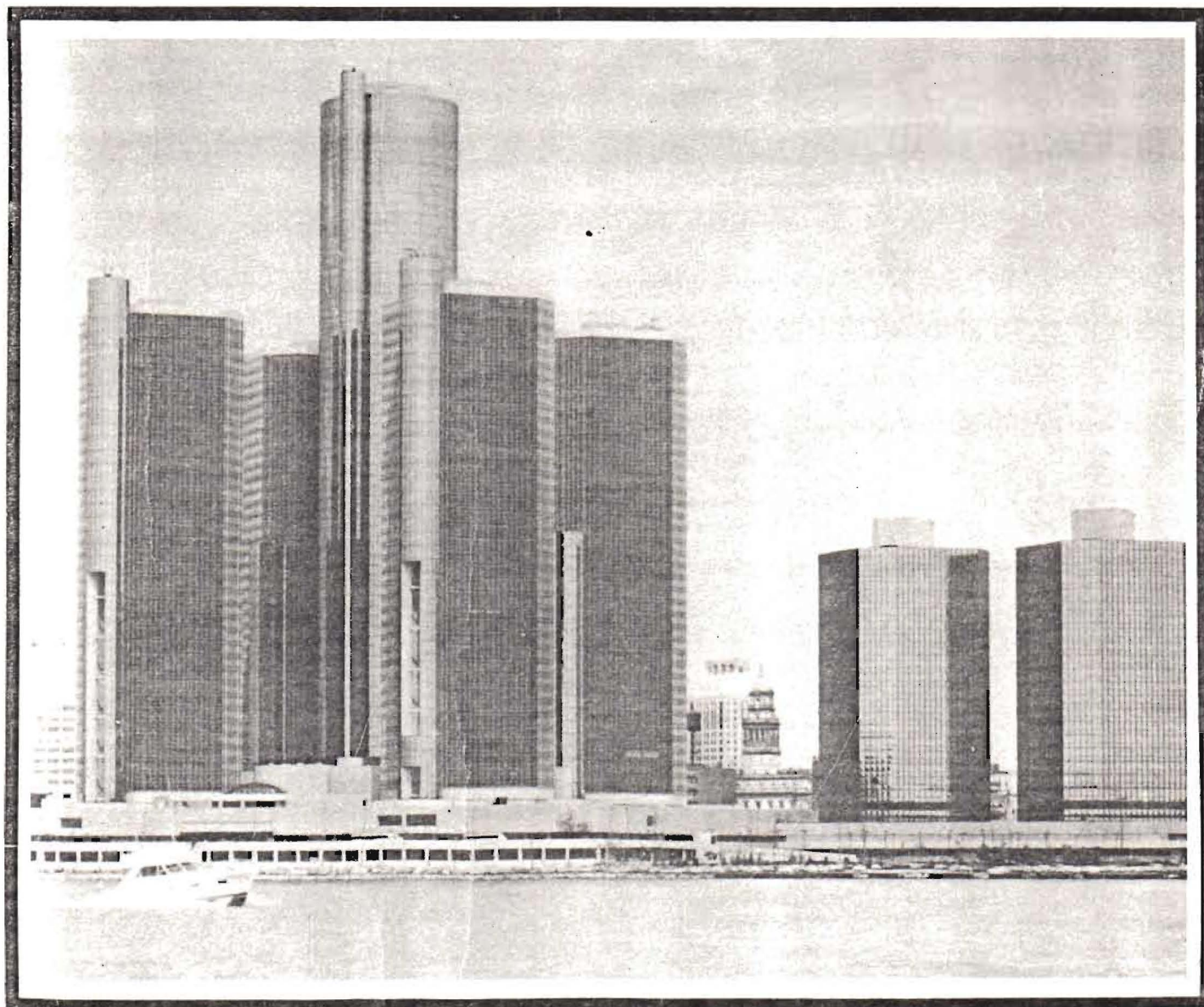
¹P. M. Grant, J. Physique 44 (Colloque C3), 847 (1983).

(X) Prefer Standard Session

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Bulletin of the American Physical Society

**Program of the 1984 March Meeting
in Detroit, Michigan; 26-30 March 1984**



U65-IRM-17

Wednesday Morning

rows as the conductivity increases but which weakens rapidly below T_M . A weak residual resonance is observed at helium temperatures in the FSO_3^- salt but not in the case of $F_2PO_2^-$. The g-tensors are unusual, being axially symmetric in both cases and with a much reduced perpendicular shift in the $F_2PO_2^-$ salt, perhaps indicative of reduced spin density at the cation Se atoms.

11:00

GE 11 Resistivity Measurements on Single Crystals of HMTSF-TCNQ as a Function of Pressure to 7.0 GPa.*

S.W. TOZER, and D.O. COWAN, Johns Hopkins U., and H. KING, J.P. STOKES, and A.N. BLOCH, Exxon Research and Engineering Co.--Pressure significantly modifies the electronic properties of organic one dimensional conductors. Moderate pressures increase conductivity, but higher pressures are predicted to produce an insulating state. Two-probe, quasi-hydrostatic measurements to 7.0 GPa on single crystals of HMTSF-TCNQ are reported. A modified diamond anvil cell generated pressures which were monitored using the standard ruby manometer. This method affords an opportunity to explore a pressure region previously unattainable with these fragile crystals. The conductivity data for HMTSF-TCNQ up to 3.0 GPa agrees with that data reported by Jérôme, et.al.** Conductivity as a function of pressure of this salt and other organic salts above 3.0 GPa shall be compared and discussed.

*This work was supported by an Industry/University Cooperative Research Activity NSF Grant DMR 8307693.

Jérôme, D., Schulz, H., 1982, Adv. in Physics, **31, 299.

11:12

GE 12 Compressibility of HMTSF-TCNQ for Pressures Up to 5 GPa.

H. E. KING, JR., Exxon Res. & Eng. Co., Annandale, N.J. 08801 -- In seeking to understand the pressure dependence of the highly anisotropic interactions in quasi-1D materials, anisotropic compressibility values are needed. Also, non-linearity in the compression makes their pressure derivatives important. The room-temperature compressibility of HMTSF-TCNQ has been measured using x-ray scattering techniques on a single-crystal sample subjected to hydrostatic pressures. At zero-pressure the stacking axis is the most compressible, but its compressibility is one-half that for the same axis in TTF-TCNQ. The anisotropy is relatively small, 1:0.6:0.5, and decreases further with increasing pressure. Analysis of the P-V data shows the bulk modulus and its pressure derivative to be, respectively, 12.2 GPa and 5.8. This is a typical value for dB/dP ; thus the degree of P-V curvature is normal. However, the high compressibility of this material makes the effect of this curvature important in calculating any strain-dependent property. For example, at elevated pressures the band-broadening component [1] of dk_f/dP is reduced by an order-of-magnitude from its zero-pressure value.

[1] Tiedje et al., S. S. Com. **23**, 713, (1977).

11:24

GE 13 Localization Effects in an Unusual Member of the (TMTSF)₂X Family of Organic Metals.

R. M. BOYSEL, D. MOSES, S. COX, F. WUDL and A. J. HEEGER, Institute for Polymers and Organic Solids, UCSB, Santa Barbara, CA.-- A metal-insulator transition has been observed in $(TMTSF)_2F_2PO_2$ which is only incompletely suppressed by high pressures. In the conducting regime at high P we find an unusual increase in $\rho(T)$ at temperatures below 20 K which may be the result of disorder induced localization arising from strong electronic scattering from the randomly oriented $F_2PO_2^-$ dipole moments. We report the results of studies of the temperature and electric field dependence of the resistivity at low temperatures. The results are discussed in the context of localization phenomena.

11:36

GE 14 Magnetic Field Dependent Susceptibility of (TMTSF)₂ClO₄*

A. FELDBLUM, A.J. EPSTEIN, Xerox Webster Research Center, R. Greene, IBM San Jose Research Lab., and P.M. CHAIKIN, Univ. of Penn.--The magnetic susceptibility of slowly cooled single crystals of $TMTSF_2ClO_4$ was measured for

$H//c$ with fields up to 10 Tesla and $1.7 \lesssim T \lesssim 300K$. No anomaly in χ is observed at the anion ordering temperature 24K, with $\chi^{Pauli} = \text{constant}$ for $4.2 < T < 30K$. Between 4.2K and 2.2K χ^{Pauli} increase threefold in agreement with the high field specific heat data. $\chi(H)$ at 4.2K and 2K shows the presence of $\sim 750\text{ppm}$ Curie spins. Such localized spins and their associated Schottky anomaly can account for a large part of the 2 Tesla low T specific heat anomaly reported earlier. Supported in part by U.S. NSF Solid State Chemistry Grants DMR-8218021 and DMR-8115241.

¹ R. Brusetti et al., J. de Physique Colloque **44-C3**, 1051 (1983).

11:48

GE 15 Band Structure Parameters of BEDT-TTF Charge Transfer Salts.

P. M. GRANT, IBM Research Laboratories, San Jose-- We have estimated the important transfer integrals for several (BEDT-TTF) compounds from dimer splittings computed in the Mulliken-Wolfsberg-Helmholtz approximation. For the 2:1 salt containing ReO_4^- , which is superconducting, we find an average anisotropy $t_{\parallel}/t_{\perp} \approx 5$, with $\langle t_{\parallel} \rangle \approx 250$ meV. Thus this compound has the lowest anisotropy of any known superconducting charge transfer salt, a result of the optimization of a key interchain interaction predicted earlier for the 2:1 salts of TMTSF.¹

¹P. M. Grant, J. Physique **44** (Colloque C3), 847 (1983).

SESSION GF: AMORPHOUS Se, Te, C;

AND CLASSICAL LIQUIDS

Wednesday morning, 28 March 1984

Marquette A Room at 9:00

P. Boolchand, presiding

9:00

GF1 The Ionic Self-Energy Contribution to the Liquid Metal Surface Energy.

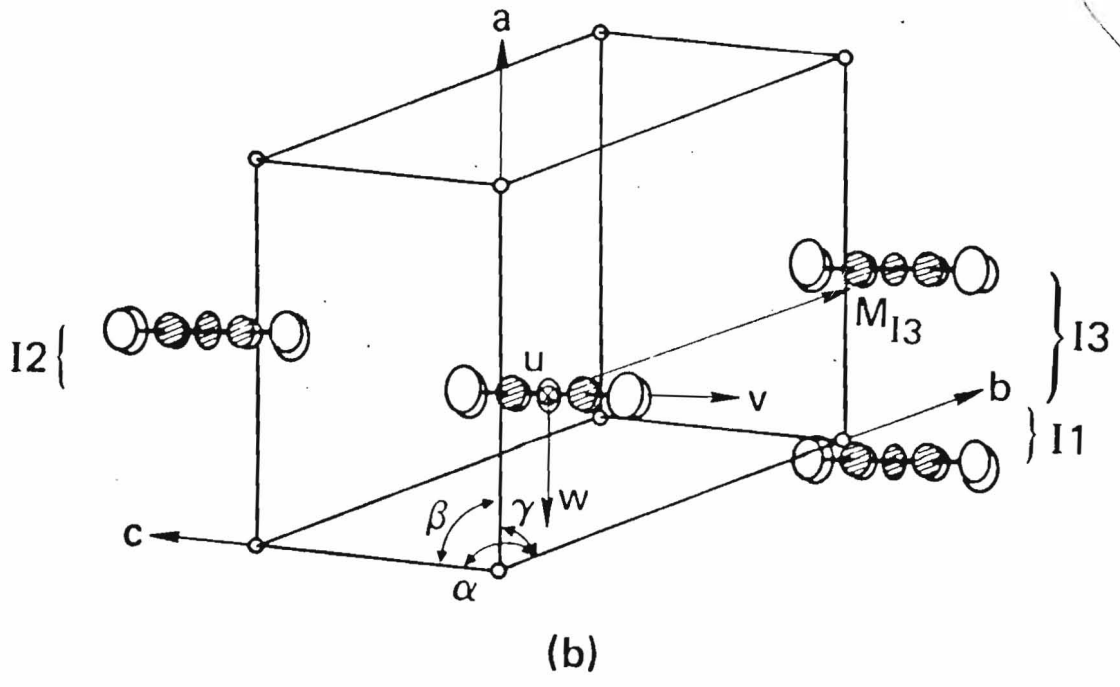
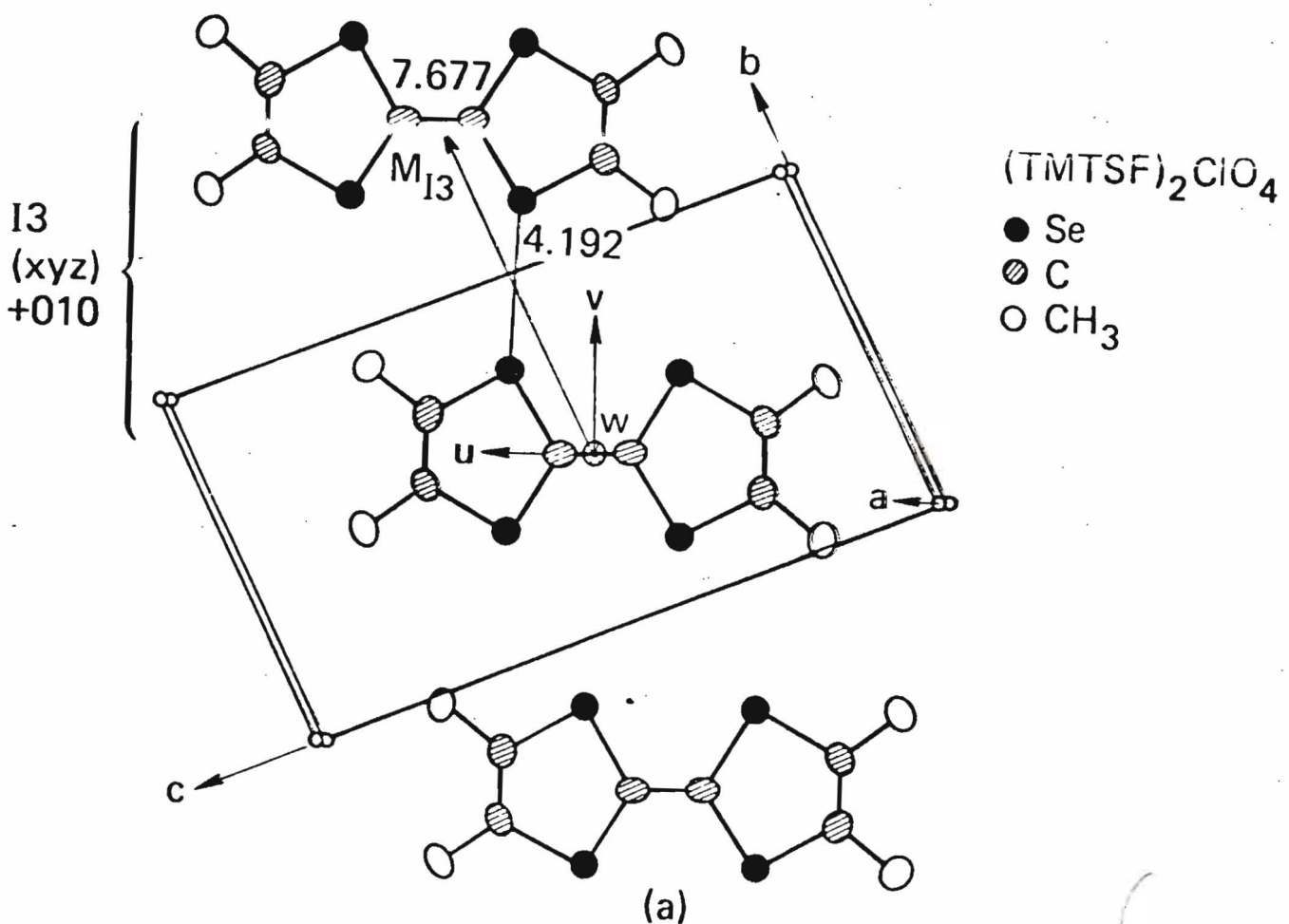
S.M. Foiles, Sandia Nat. Labs., and N.W. Ashcroft, Cornell U.*--The surface energy of liquid simple metals has been computed by various authors using pseudopotential perturbation theory about a non-uniform electronic density appropriate to the surface. The energy is then readily decomposed into a sum of the electron gas energy, an ionic self-energy, and position dependent pair interactions. The second order or screening contribution to the self energy is usually taken to be the screening energy of an ion in a uniform electron gas with the local electronic density. This last approximation is examined here using various simple models of the response function of an inhomogeneous electron gas. The results indicate that the local approximation is quantitatively poor for the polyvalent metals and that the use of the local approximation may account for many of the difficulties found in using the perturbation approach for the surfaces of polyvalent simple metals.

*Supported by NSF Grant DMR-80-20429

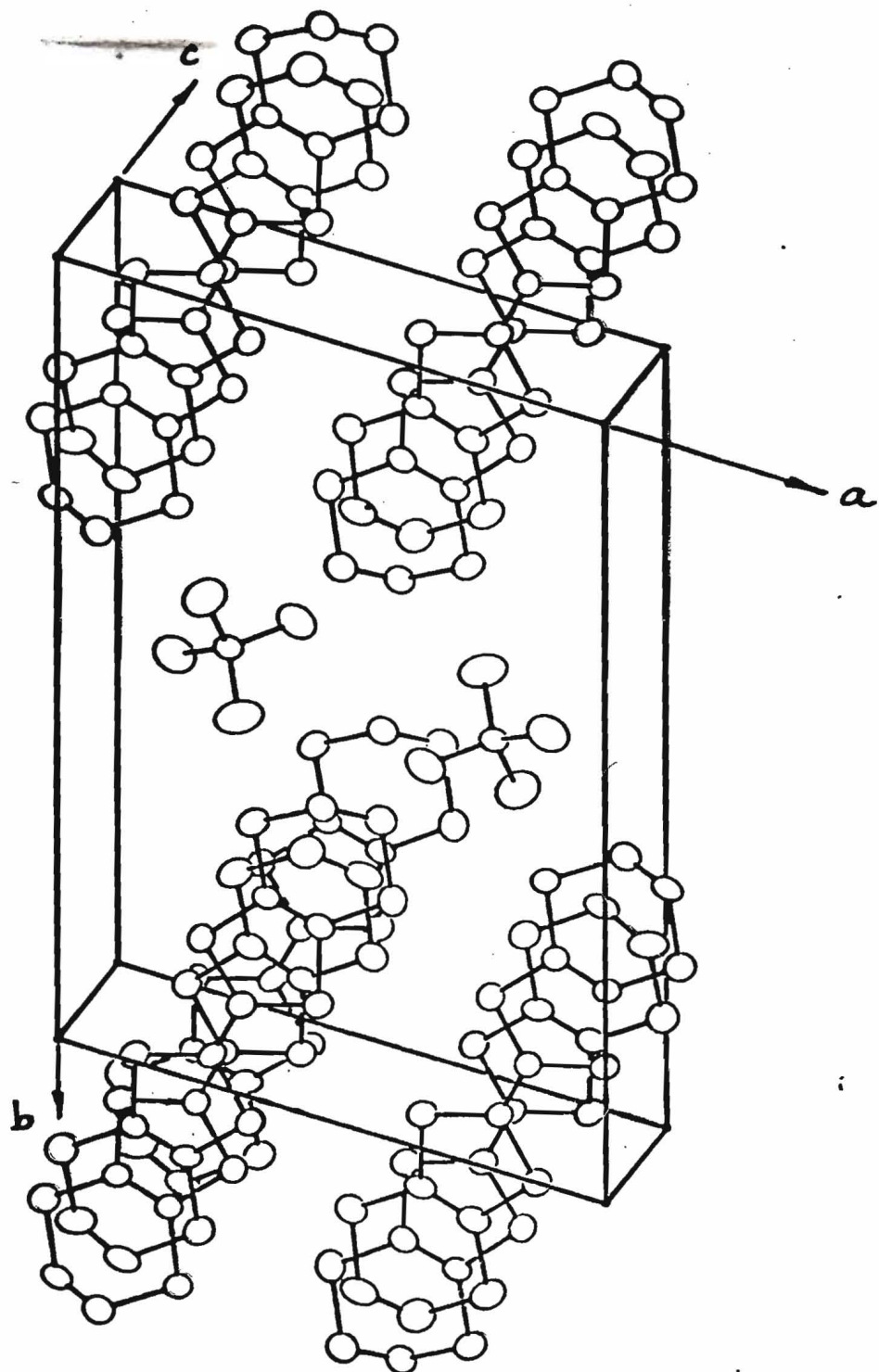
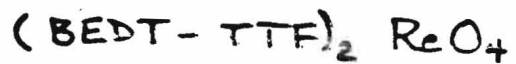
9:12

GF2 Short Range Order in Amorphous Se and Te with Dilute In Impurities, J. A. GARDNER and D. K. GASKILL, Oregon State U.*--The time differential perturbed angular correlation (TDPAC) technique was used to measure the distribution of electric field gradients at the site of a ^{111}Cd nucleus in splat-quenched amorphous Se and Te.

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$$H_e(p'_j, p_j) = K S_e(p'_j, p_j) [E_{p'_j} + E_{p_j}] / 2$$

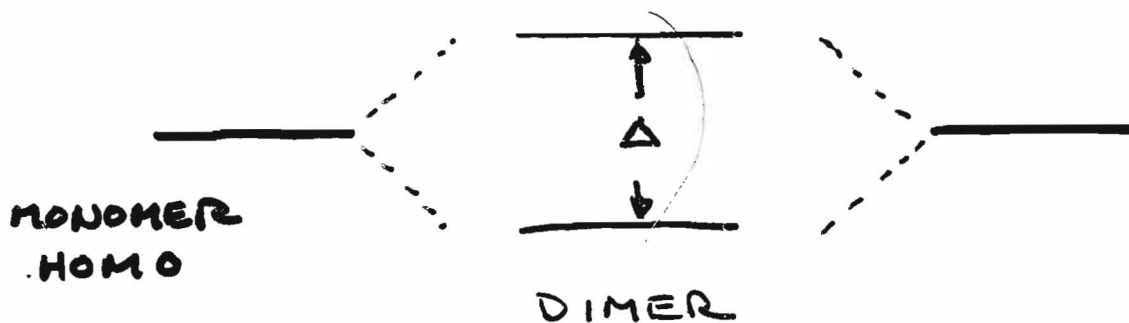
BASIS SET

$$\psi_{nlm} = R_{nl}(r) Y_{lm}(\theta, \phi)$$

$$R_{nl}(r) = \sum_{\lambda(0)} C_{n_\lambda} [(2n_\lambda)!]^{-1/2} (2\zeta_\lambda)^{n_\lambda + 1/2} \\ \times r^{n_\lambda - 1} e^{-\zeta_\lambda r}$$

TRANSFER INTEGRAL CALCULATION

- CONSIDER EACH PAIRWISE INTERMOLECULAR INTERACTION INDEPENDENTLY (DIMERS)
- TAKE EACH TRANSFER INTEGRAL AS ONE-HALF THE APPROPRIATE DIMER SPLITTING OF THE MONOMER HOMO:

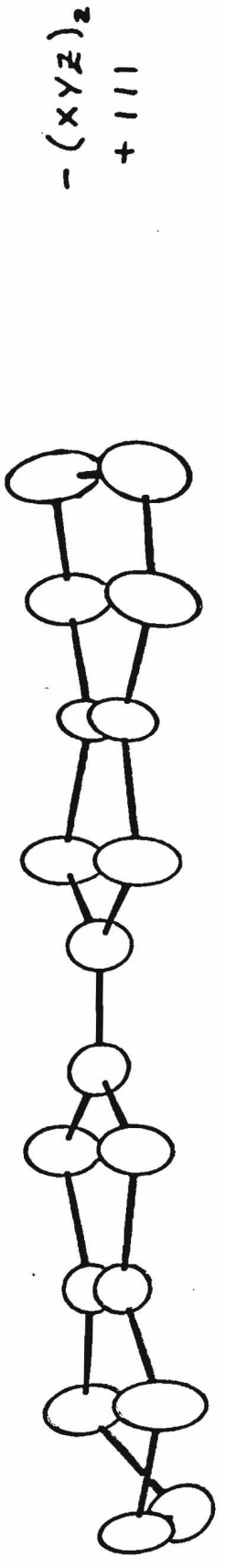


$$\text{BANDWIDTH} \approx 2\Delta$$

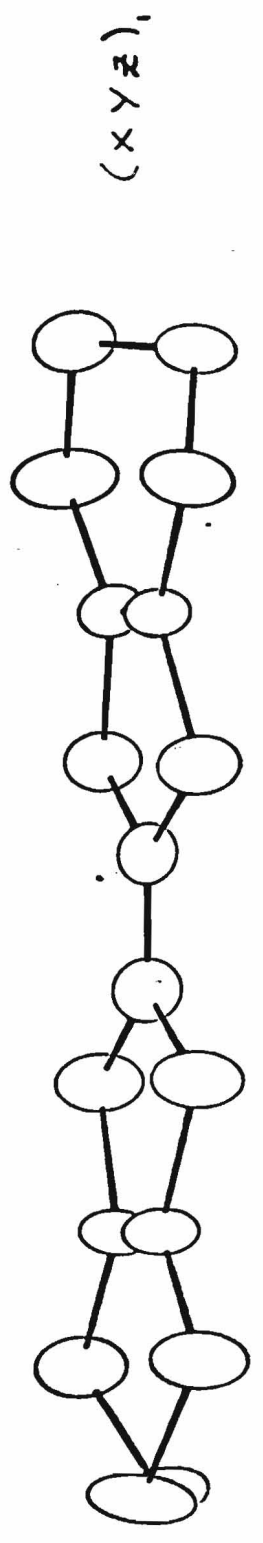
$$\therefore t \approx \Delta/2$$

- COMPARE WITH "FULL" MWH BAND STRUCTURE CALCULATION

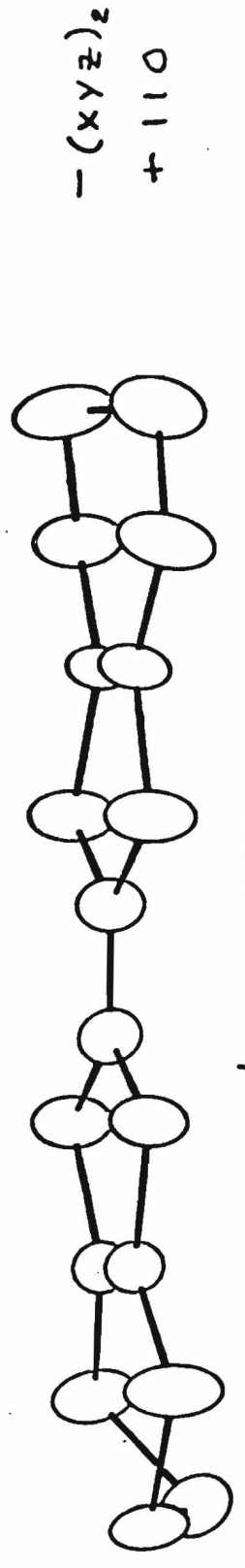
S1 & S2 INTERACTIONS



S1: 3.597



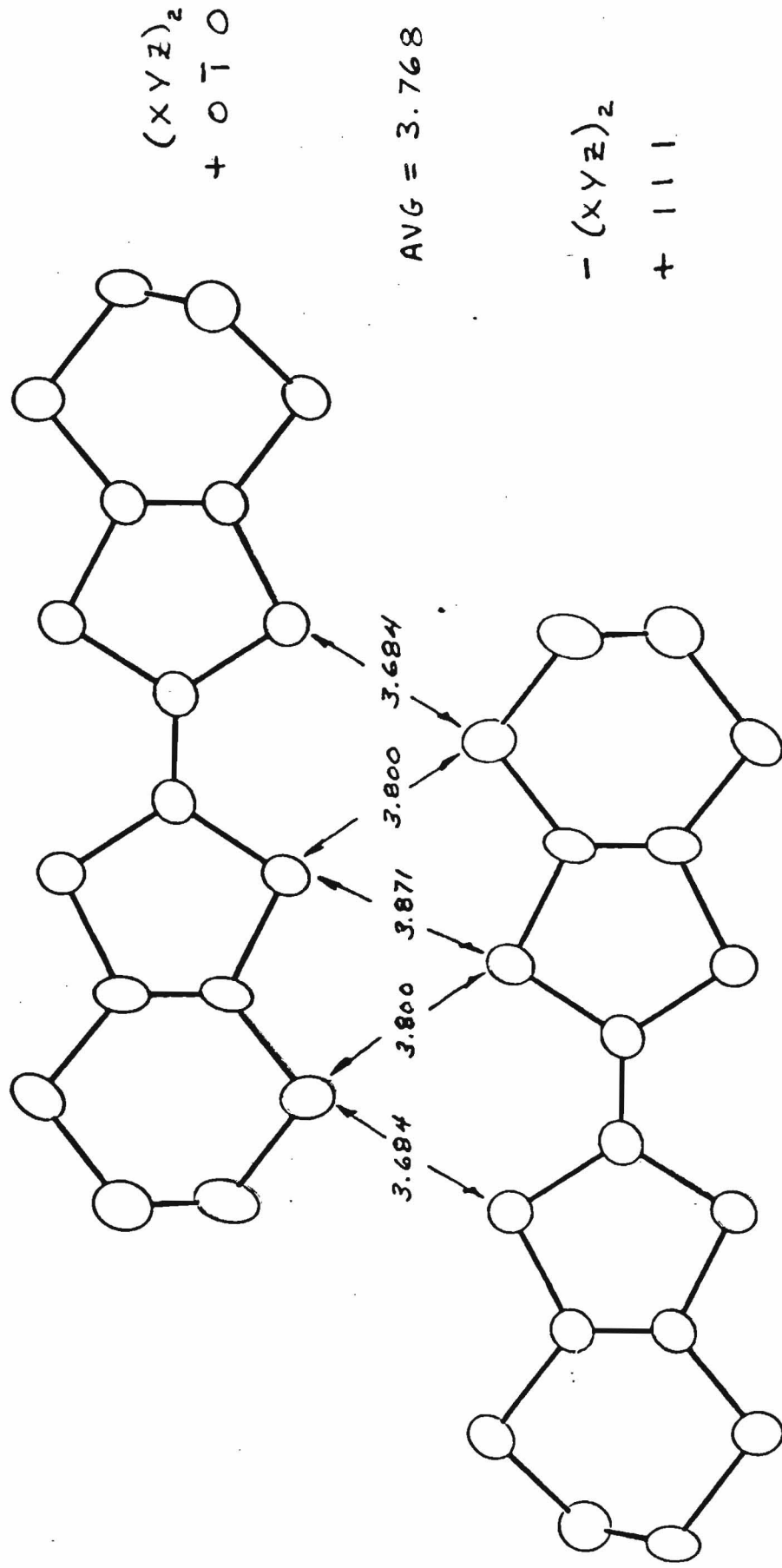
S2:



$t_{s1} = 263 \text{ meV}$

$t_{s2} = 243 \text{ meV}$

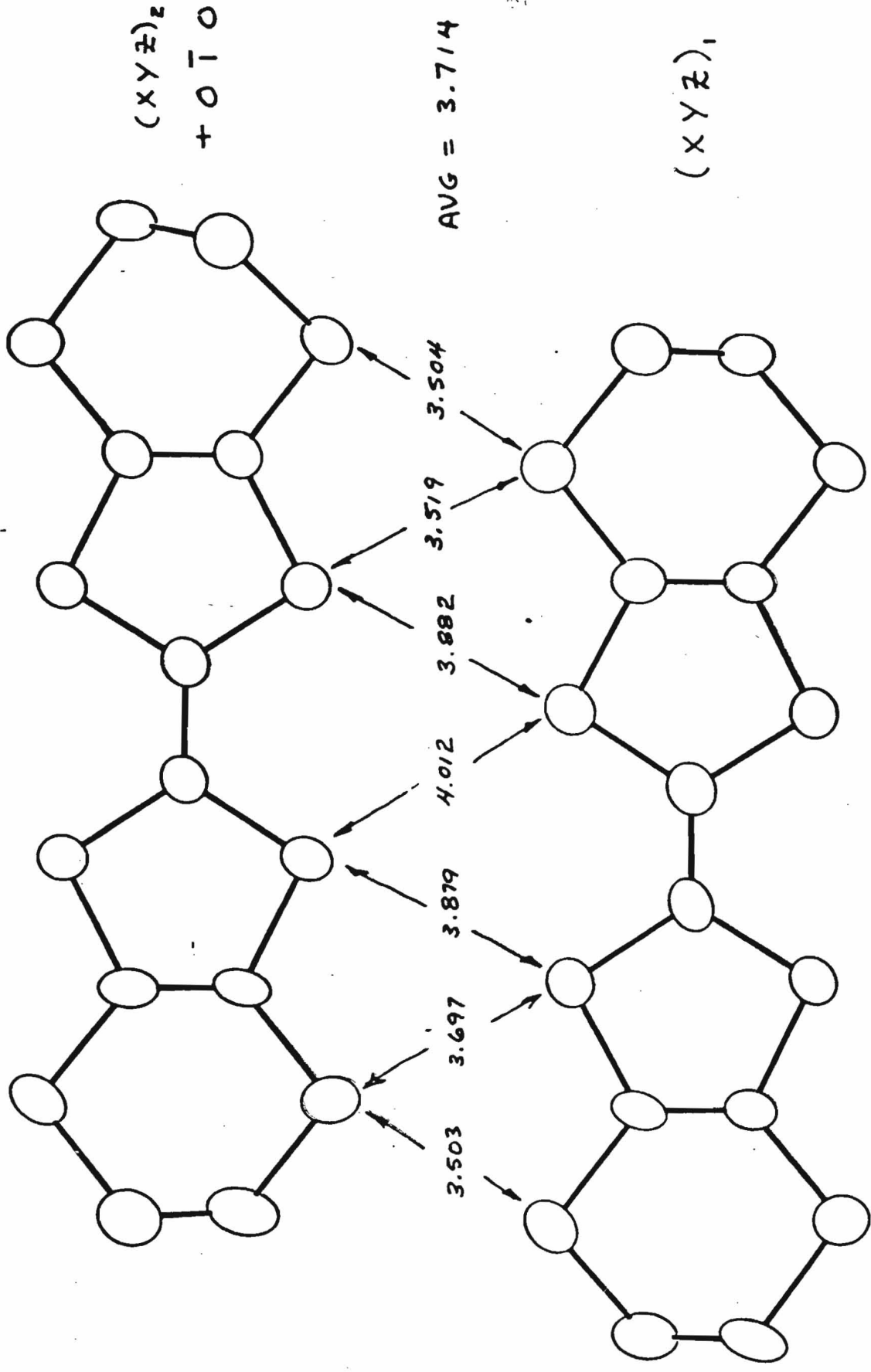
I 2 INTERACTIO



$$t_{I2} = 46 \text{ meV}$$

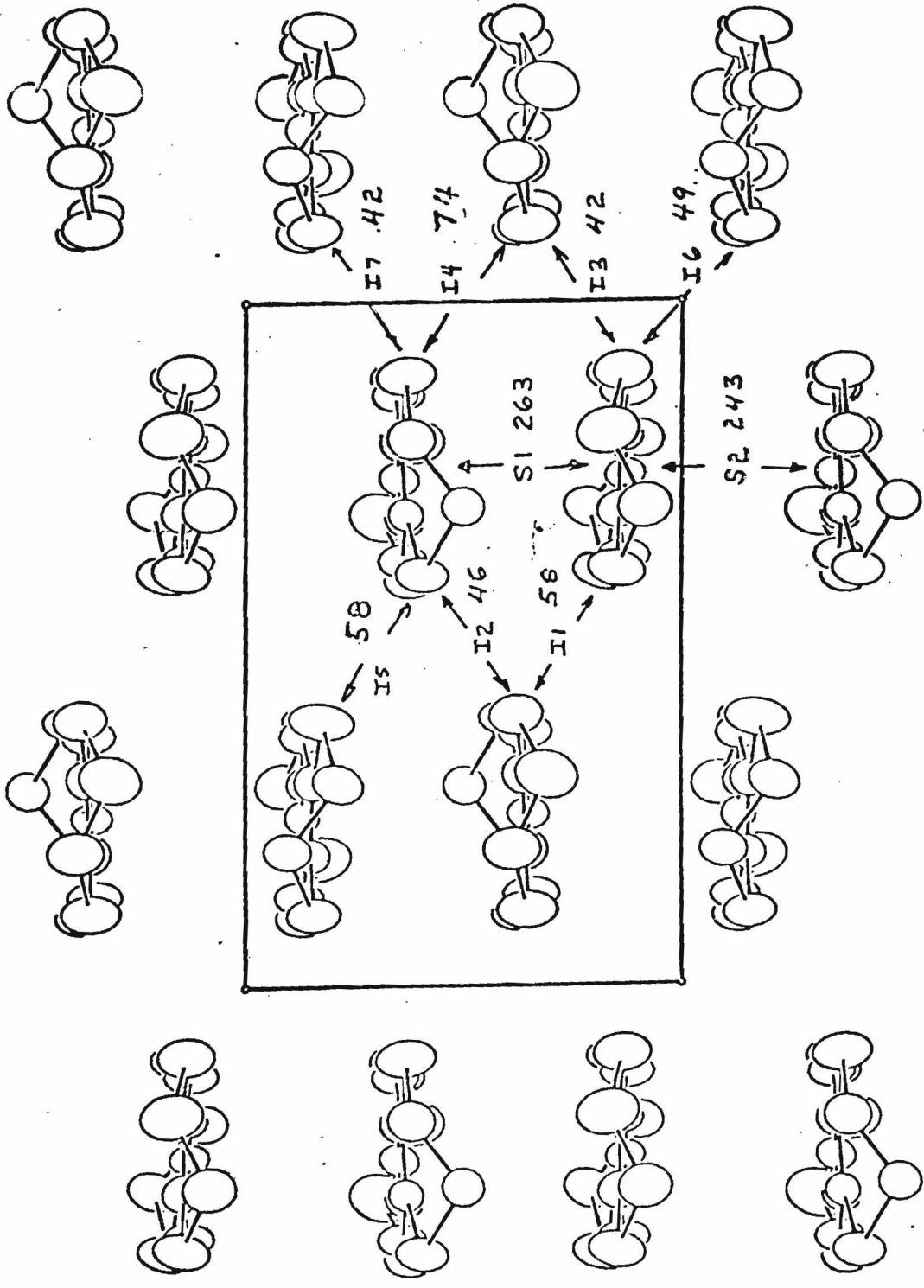
II INTERACTION

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IBM

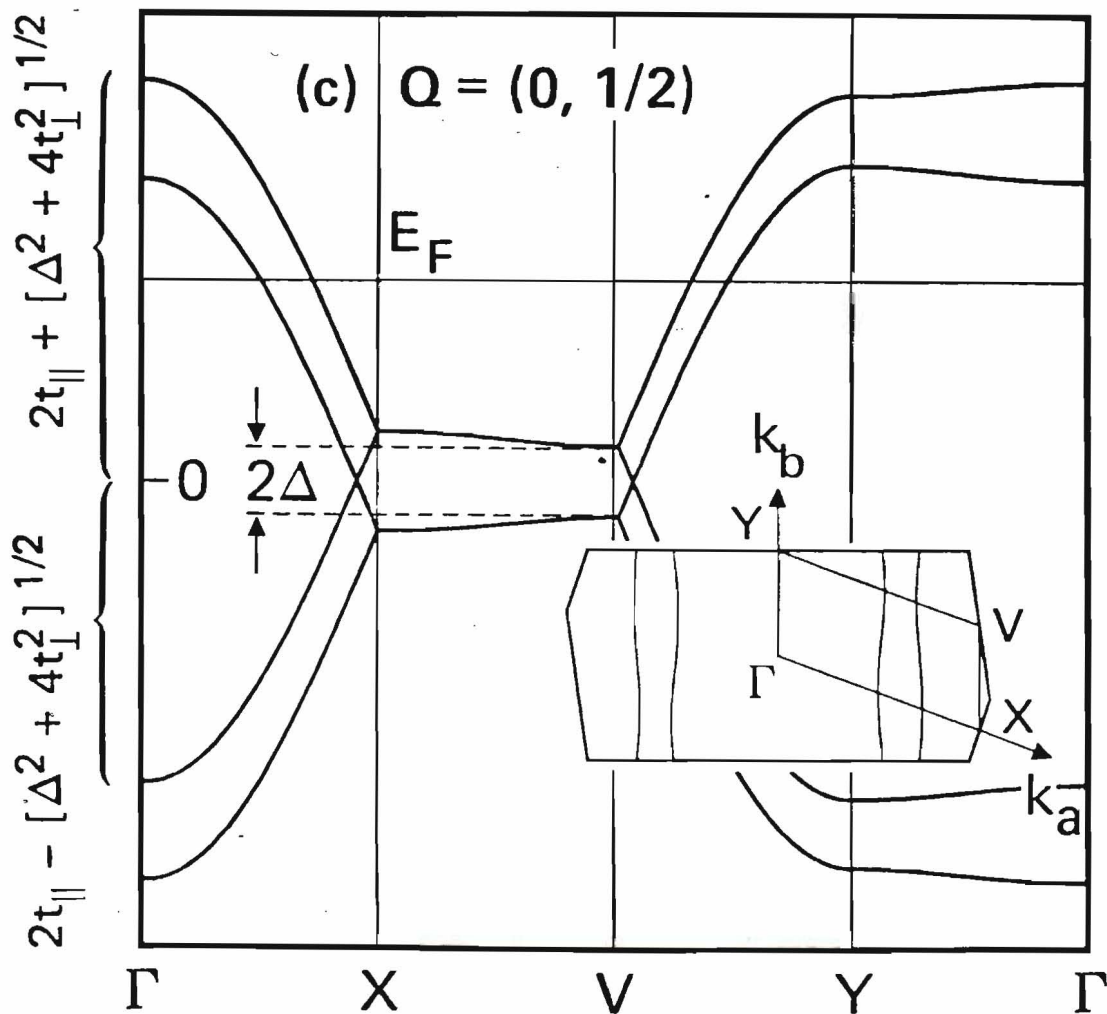


$t_{I1} = 58 \text{ meV}$

(BEDT-TTF)₂ ReO₄ CATION INTERACTIONS



ALL INTERSTACK INTERACTIONS I3 - LIKE



- NO GAPS FOR ANY FINITE 2Δ
(ALWAYS METALLIC)
- FOUR FERMI CONTOURS
- RELAXED CrO_4 : SDW SUPPRESSED
BY INCOMMENSURABILITY
- $(\text{BEDT-TTF})_2 \text{ReO}_4$

CONCLUSIONS

• Transfer Integral Summary

	t_s	t_x	t_s/t_x
$(\text{TMTSF})_2 \text{X}$	370	23	16
$(\text{TMTTF})_2 \text{X}$	220	11	21
$(\text{BEDT-TTF})_2 \text{ReO}_4$	253	46	5

• $(\text{BEDT-TTF})_2 \text{ReO}_4$ is the most 2D CT salt known

• $(\text{BEDT-TTF})_2 \text{ReO}_4$ has a band structure much like relaxed $(\text{TMTSF})_2 \text{ClO}_4$ and $(\text{TMTSF})_2 \text{ReO}_4$