Crystallographic Studies of Iodide-Containing Quasi-One-Dimensional Conductors

Thesis by

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In Partial Fulfillment of the Requirements

for the Degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California

1980

(Submitted June 20, 1979)

Acknowledgements

I would like to thank Dr. Joseph Gordon for initially interesting me in the field of quasi-one-dimensional conductors and for his continued interest in the research.

Dr. Sten Samson, my advisor, spent many invaluable hours explaining the "care and feeding" of X-ray diffraction equipment to me. The low-temperature studies of TTT_2I_3 would not have been possible without his new low-temperature goniometer. He also provided much encouragement.

Dr. Richard Marsh was very helpful with the interpretation of Patterson maps. He was also quite helpful with some of the subtleties of data collection and structure refinements. Without Jean Westphal's aid the computing so necessary for this research would have been torturous.

This research has been conducted in collaboration with the organic metals group at JPL. Dr. Robert Somoano and Dr. V. Hadek supplied the TTT_2I_3 and TTTI crystals for this research. All of the transport properties were measured by the group at JPL. I would like to thank Dr. Robert Somoano for many interesting and helpful discussions.

I would also like to thank Beth Cooper for typing this thesis. Pat Anderson and Allison Kimball have also been very helpful during the past five years. The staff at Caltech have helped make doing research here much easier.

Roger Williams has been a good friend and invaluable research companion. His chemical intuition and assorted wild theories have

helped to keep me "chemically honest" and provided the starting point for many interesting discussions. He also provided the HMTSF-I_x crystals.

My parents, brother and sister, and my in-laws have all provided a great deal of encouragement and support during the past five years.

Funding for this research came from a variety of sources including NASA-JPL and NSF (Grant No. DMR74-19029A1). Eastman Kodak and IBM provided fellowship support.

Finally, I would like to thank my husband Hamil Ma. He prepared all of the figures in this thesis. He also helped with the low-temperature runs whenever I was too tired to be lucid. Hamil has been the ideal husband and without him the last few years would have been unbearable.

Abstract

The crystal structures of three iodide-containing quasi-one-dimensional conductors, (tetrathiotetracene)$_2$(iodide)$_3$ (high disorder), tetrathiotetracene-iodide, and (hexamethylenetetraselenofulvalene)-(iodide)$_x$ were solved by single crystal X-ray diffraction methods. These three iodides are single charge-carrier conductors and allow a comparison of such competing effects as disorder, interchain coupling, and overlap.

The crystal structure of metallic (tetrathiotetracene)$_2$(iodide)$_3$ (high disorder), TTT_2I_3 (h.d.), was solved at room temperature (~294° K), 164° K, 74° K, and at 19° K. At all four temperatures the lattice symmetry remained orthorhombic and the structures were successfully refined in the space group Cmca. During slow cooling the diffuse layer lines were also carefully monitored. In contrast to $TTFCl_{0.67}$, even with slow cooling the iodide chains do not three-dimensionally order, and there are no distortions in the TTT lattice to 19° K. A model of the iodide chains is presented which explains the positions and intensities of the diffuse layer lines and also explains why three-dimensional ordering at low temperatures is not observed.

The structure of semiconducting tetrathiotetracene-iodide (TTTI) was studied at room temperature. The structure consists of two ordered lattices which are incommensurate along $\vec{c}$, the stacking axis. The unit cell dimensions for Lattice 1 (triclinic, $C\bar{1}$) are a = 13.028(2), b = 16.445(2), c = 3.643(1) Å and α = 90.81(1)°, β = 96.11(1)°, and γ = 91.11(1)°.

For Lattice 2, c ≃ 4.78 Å. The positions of all of the layer lines, including the two "sixth" layer lines, which are observed on X-ray oscillation photographs of crystals of TTTI rotated about $\vec{c}$, can be explained by the presence of two lattices. The measured density $d_m \simeq 2.09$ g/cm^3 and refinement of the [001] projection (hk0 reflections) confirmed that the overall stoichiometry is TTTI (1:1). For a complete data set collected with copper K_α radiation, the refinement of Lattice 1 converged to R = 0.102. For the 1132 reflections with $F_o^2 > 3\sigma(F_o^2)$, R = 0.081. The overlap between adjacent TTT cations in the same stack in TTTI is significantly different from that observed in TTT_2I_3 (h.d.). There is also very little interchain coupling in TTTI.

Hexamethylenetetraselenofulvalene-iodide, HMTSF-I_x, is triclinic, $P\bar{1}$, with the unit cell parameters a = 8.056(4), b = 12.740(4), c = 8.016(3) Å and α = 81.72(4)°, β = 67.73(5)°, and γ = 102.64(4)°. For a complete data set of 4213 reflections collected with monochromatized molybdenum K_α radiation to 2θ = 60° the structure refined to R = 0.097. For 2042 reflections with $F_o^2 > 3\sigma(F_o^2)$, R = 0.051. The hydrogen atoms were not located. There is disordered iodide and solvent at 1/2,1/2,1/2. The HMTSF cations stack along $\vec{a}$. A new type of alternating overlap between adjacent HMTSF molecules was observed. The magnitude of the d.c. electrical conductivity at room temperature suggests that this phase of HMTSF-I_x is semiconducting.

These iodide-containing structures show three different types of iodide behavior in quasi-one-dimensional conductors. In TTT_2I_3 (h.d.) the slip-stacking and large interchain coupling favor formation of a

metallic state at high temperatures. At low temperatures the disordered iodide chains have a major effect on the transport properties by allowing states to exist in the semiconductor band gap. In TTTI the iodides are no longer disordered but still dominate the physical properties by causing a modulation of the TTT lattice. There is very little inter-chain coupling in TTTI. In HMTSF-I_x the iodide is probably of minor importance.

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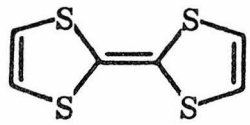
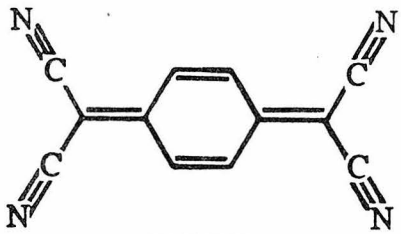
Chapter 1

Introduction

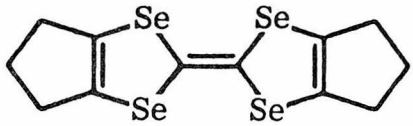
Quasi-one-dimensional conductor is a label which has been given to materials that exhibit highly anisotropic, "one-dimensional", electrical conductivity. Conduction in the perpendicular directions in these materials is usually 10^3 to 10^5 times less than along the axis of high conductivity. Conductivity is not the only anisotropic property of these materials. They also have direction-dependent optical, magnetic and mechanical properties. An example of a quasi-one-dimensional material which has been studied in great detail is tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ). TTF and TCNQ are two planar organic molecules (see Figure 1) which together form a charge-transfer complex. TTF is an electron donor and TCNQ is an electron acceptor. In crystals of the complex the TTF molecules are stacked on top of each other and next to the TTF stacks are stacks of TCNQ molecules. The significance of this arrangement is that the TTF molecular orbitals are spatially close and it is energetically favorable for intermolecular orbital interaction and the formation of a "band". The TCNQ molecules also stack and the molecular orbitals also form a "band". Because there is charge transfer between the TTF and TCNQ molecules the bands become only partially filled and TTF-TCNQ exhibits metallic conductivity and metallic behavior parallel to the stacking direction. Conductivity parallel to the stacking direction is ~500-700 Ω^{-1} cm^{-1} at room temperature and ~5 Ω^{-1} cm^{-1} perpendicular to the stacking



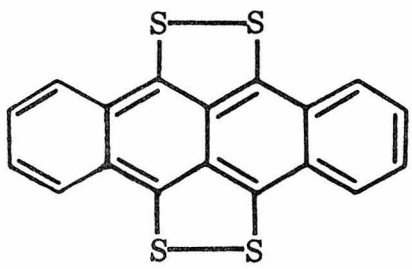
TTF



TCNQ



HMTSF



TTT

Figure 1

direction (1). Many quasi-one-dimensional conductors formed from organic donor-acceptor complexes with similar arrangements of separate cation and anion stacks are known (1). The best organic quasi-one-dimensional metal known is hexamethylenetetraselenofulvalene-tetracyanoquinodimethane (HMTSF-TCNQ) (2). It has a room temperature conductivity of ~2000 Ω^{-1} cm^{-1} and, in contrast to TTF-TCNQ which undergoes a phase transition to an "insulating" state, HMTSF-TCNQ remains highly conducting to below 1° K (2). For comparison, copper, a good three-dimensional metal, has a conductivity of 5.88 x 10^5 Ω^{-1} cm^{-1} at 295° K (3). Liquid mercury, a poor three-dimensional conductor, has a conductivity of ~10000 Ω^{-1} cm^{-1} at 295° K (3).

The conductors formed from organic donor-acceptor charge-transfer complexes, such as TTF-TCNQ and HMTSF-TCNQ, are two-carrier systems. Electrons are conducted along the anion stacks and holes along the cation stacks. This makes the interpretation of their properties complex. The properties of single charge-carrier systems, in principle, are easier to interpret. Studies of single charge-carrier systems help toward a better understanding of the effect of disorder, impurities, intermolecular overlap, and interchain coupling. The TTF halides and pseudo-halides (SCN^-, $SeCN^-$) have been extensively studied for these reasons (for example 4,5,6,7,8).

The interpretation of solid-state physical properties ultimately depends on a knowledge of the underlying crystal and molecular structure. Although X-ray diffraction always emphasizes crystalline perfection, it is a convenient method for determining the actual internal structure

of a crystal. X-ray diffraction studies of the iodides of HMTSF and tetrathiotetracene (TTT) (Figure 1), which are single charge-carrier quasi-one-dimensional conductors, were undertaken to determine their stoichiometry, the role of disorder, the effect of variations in intermolecular overlap and interchain coupling, and in the case of the temperature-dependent structural studies of TTT_2I_3 the nature of its phase transitions.

All of the crystallographic data reduction and structural computations necessary for this study were done with the CRYM crystallographic computing system and an IBM computer 370/3032.

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Chapter 2

Temperature-Dependent Studies of Highly-Disordered (Tetrathiotetracene)$_2$-(Iodide)$_3$

Introduction

Tetrathiotetracene* (TTT) is a planar organic molecule which as long ago as 1965 was known to form organic donor-acceptor charge-transfer complexes (1,2). These early charge-transfer complexes had resistivity values of 2-15 Ω cm. Although Marschalk and coworkers were the first to report the syntheses of ion-radical salts of TTT (3,4), Perez-Albuerne and coworkers reported in 1971 that the halide and thiocyanate salts of TTT formed highly conducting powders (5). The iodide salt, of poorly defined stoichiometry, had a powder resistivity of 0.71 Ω cm. Eventually single crystals of TTT_2I_3 were grown and temperature-dependent conductivity measurements indicated that TTT_2I_3 was metallic (6,7). Additional electrical, magnetic, and optical studies of crystals of TTT_2I_3 grown at the Jet Propulsion Laboratory (JPL), Pasadena, have shown that for temperatures of $100° < T < 300°$ K TTT_2I_3 is metallic (8). The d.c. conductivity at room temperature is about 1000 Ω^{-1} cm^{-1} parallel to the crystal needle axis. At about 100° K abrupt changes in the conductivity, ESR linewidth, and thermoelectric power (TEP) suggest that a phase transition has occurred.

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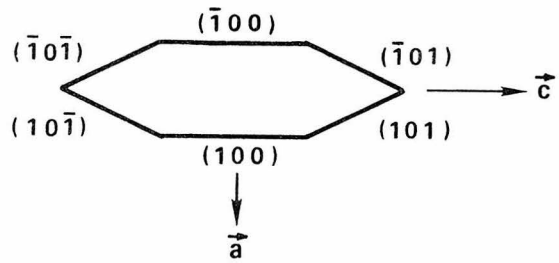
*naphthaceno[5,6-cd:11,12-c'd']bis[1,2]dithiole.

Below 20-30° K the electrical and magnetic properties indicate that TTT_2I_3 has undergone an additional phase transition to a nonmetallic state (8).

The basic structure of TTT_2I_3 is known at room temperature (6,9). However, temperature-dependent structural information would clarify the nature of the phase transitions at ~100° K and ~20°-30° K and would help clarify the role of disorder. For these reasons, an extensive temperature-dependent X-ray diffraction study of TTT_2I_3 was undertaken.

Single crystals of TTT_2I_3 are grown from hot nitrobenzene solutions of TTT and iodine (I_2) by slow-cooling (V. Hadek and R. B. Somoano, JPL). TTT_2I_3 crystals are long, dark, well-formed, six-sided orthorhombic needles which give golden reflections off the faces. The needle axis, the axis of high conductivity, is $\vec{b}$. For a C-centered TTT lattice, the crystallographic axes and the indices of the faces are oriented as shown below. ($\vec{b}$ is perpendicular to the page.) The a and c axes



have almost the same lengths but can be distinguished because the 800 and $00^{1}2$ are weak reflections whereas the $^{1}200$ and 008 are both strong reflections. Two general features of X-ray oscillation photographs of crystals of TTT_2I_3 rotated about $\vec{b}$ are the presence of layer lines with three-dimensional Bragg diffraction spots and the presence of

several incommensurate diffuse layer lines. (See, for example, Figure 15.) The lattice giving rise to the three-dimensional diffraction spots is referred to as the TTT lattice. However, this is not meant to imply that only the TTT molecules contribute to the diffraction pattern. By just slightly varying the crystallization conditions, crystals of TTT_2I_3 with varying amounts of disorder can be obtained. The variations in disorder, as observed by X-ray diffraction, have been correlated with observed variations in conductivity and thermoelectric power measurements (10, Appendix A). The variations in the amount of disorder can be determined, with oscillation photographs or diffractometer scans, by the variation in beading or diffuseness of the strongest diffuse layer line. At room temperature the highly-disordered material, TTT_2I_3 (h.d.) has very little beading on the strongest diffuse layer line. Crystals of TTT_2I_3 (h.d.) were obtained from JPL for the temperature-dependent structural studies reported here.

2.1 Room Temperature Structure

Experimental

A crystal of TTT_2I_3 (h.d.) with the dimensions 0.06 x 0.123 x 0.60 mm was used for room temperature data collection. Unit cell parameters for the TTT lattice were obtained from a symmetry-constrained (orthorhombic) least-squares fit of the angular settings (2θ, ϕ, χ) of ten reflections carefully centered with a beam splitter (Table I). The room temperature data were obtained with nickel-filtered copper K_α radiation on an automatic, General Electric, quarter-circle diffractometer. Intensities were collected with 1° per minute 2θ-θ scans. Backgrounds were collected for 20 seconds on each side of the scans. The integrated intensities were corrected for Lorentz and polarization effects. Weights were based on counting statistics and corrected for proportionality error (11). No more than two observations contributed to a weight. Absorption corrections based on a rectangular solid (μ = 274.108 cm^{-1}) (12) were applied to the data (13). The final, complete data set for the TTT lattice consisted of 919 reflections of which 713 reflections had $F_o^2 \geq 3\sigma(F_o^2)$. No violations of the systematic absences hkℓ, h+k odd; h0ℓ, h and ℓ odd; and hk0, h odd were observed suggesting the space group Cmca. This agrees with what Smith and Luss reported (9). Preliminary atomic coordinates were determined from a three-dimensional Patterson map. Successive improvements to the model were based on three-dimensional Fourier and difference Fourier maps. The hydrogens

Table I

Crystal Data for TTT_2I_3 (h.d.) ~294° K

a = 18.347(3) Å

b = 4.962(1) Å (λ = 1.5418 Å)

c = 18.454(3) Å

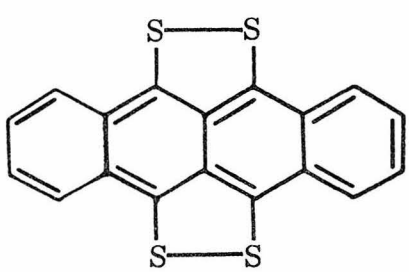
$\alpha = \beta = \gamma = 90.0°$

V = 1680.0(9) Z = 2 d_c = 2.147

Orthorhombic, Space group Cmca

Linear absorption coefficient (CuK_α), μ = 274.108 cm^{-1}

Crystal dimensions 0.123 mm X 0.60 mm X 0.06 mm

TTT ≡ 

were included in the refinement after they were observed on a difference Fourier map. After trial and error the electron density in the iodide channels was determined to be best fit by using two iodine atoms with variable populations and highly anisotropic temperature factors. The iodine atoms in the model are actually correlated because they both represent a single broad maximum of electron density and, therefore, only their populations and temperature factors were allowed to vary during refinement. The best coordinates for the iodine atoms were determined from difference Fourier sections. With the exception of the iodine atomic coordinates, all of the parameters were refined by the full-matrix least-squares method. Structure factors were calculated using the real part ($f_0 + \Delta f'$) of sulfur and iodine atomic scattering factors which had been corrected for anomalous dispersion (14). The refinement converged to R = 0.061, and the goodness-of-fit = 3.96 for the entire data set (15). For 713 reflections with $F_o^2 \geq 3\sigma (F_o^2)$, R = 0.054. A final three-dimensional difference Fourier map showed residual density ranging from -0.7e/Å^3 to +0.6e/Å^3.

Discussion

Listed in Table II are the atomic coordinates and thermal parameters for the room-temperature structure. Shown in Figure 1 is an [010] projection of the structure. The TTT molecule has 2/m symmetry and only one-quarter of the molecule is crystallographically unique. The iodine atoms are in channels which parallel $\vec{b}$. As schematically shown

Table II

Atomic Coordinates and Thermal Parameters for TTT_2I_3 (h.d.) at ~294° K (Copper K_α)

	X	Y	Z	Populations
I1	.25	.323	.25	.8426(795)
I2	.25	.198	.25	.5684(792)
C1	.03875(26)	0	0	
C2	.07609(20)	.17861(87)	.04433(21)	
C3	.03965(21)	.36659(84)	.08902(19)	
C4	.07602(25)	.55283(100)	.13418(22)	
C5	.03919(29)	.73078(106)	.17562(21)	
S	.17080(6)	.15216(28)	.03878(7)	

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I1	.0489(17)	.3425(301)	.0575(17)	0	-.0120(14)	0
I2	.0568(27)	.3680(419)	.0585(23)	0	.0289(29)	0
C1	.0337(25)	.0270(31)	.0268(21)	0	0	.0022(21)
C2	.0330(16)	.0305(26)	.0323(17)	-.0007(17)	.0007(14)	.0012(17)
C3	.0442(20)	.0280(22)	.0286(15)	-.0016(20)	-.0038(15)	.0028(16)
C4	.0517(21)	.0341(28)	.0321(17)	-.0043(22)	-.0082(17)	-.0020(18)
C5	.0774(30)	.0344(27)	.0293(17)	-.0068(26)	-.0074(21)	-.0021(18)
S	.0345(5)	.0456(7)	.0594(7)	-.0035(6)	-.0030(5)	-.0085(6)

	X	Y	Z	B
H1	.1308(32)	.5516(116)	.1279(29)	5.11(1.29)
H2	.0674(29)	.8876(106)	.2040(29)	4.68(1.25)

PROJECTION DOWN b-AXIS OF TTT_2I_3

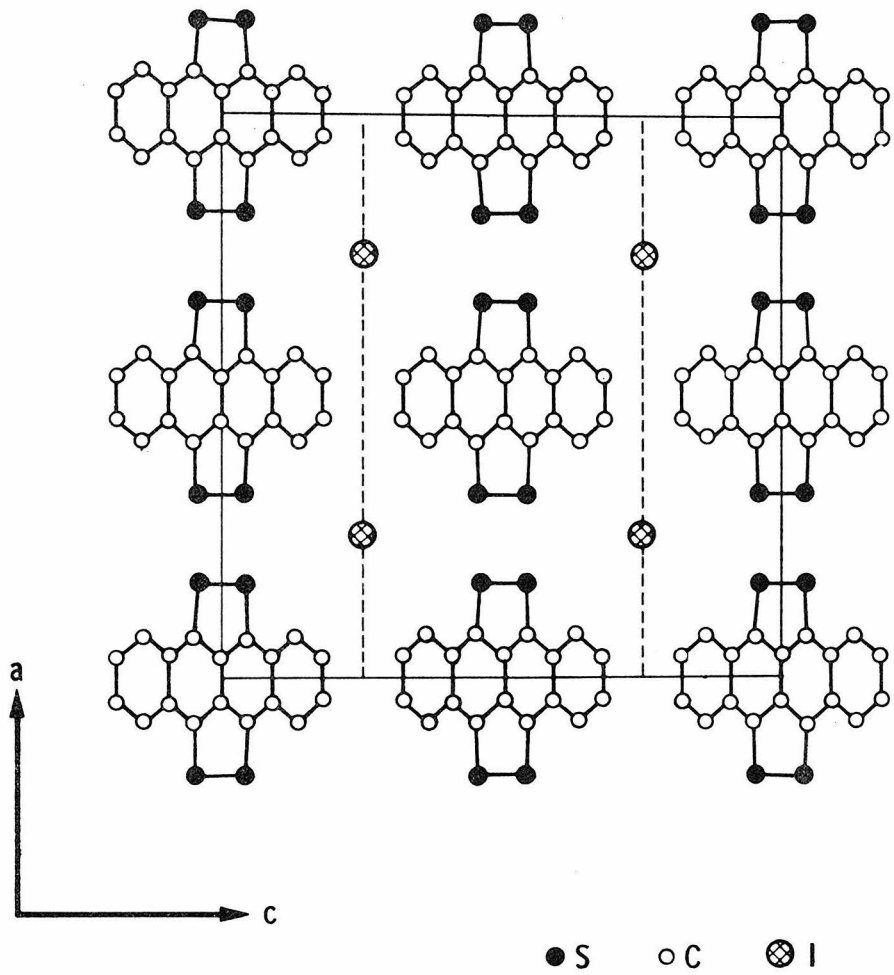
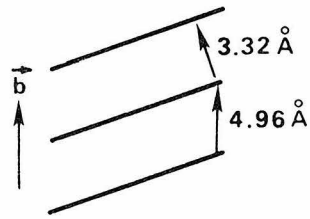


Figure 1

below, each TTT molecule is slipped with respect to neighboring molecules, but the entire stack is parallel $\vec{b}$.



There are uniform TTT-TTT spacings along the stack because a TTT to TTT translation along $\vec{b}$ defines the lattice spacing.

As can be seen in Tables III, XI and Figure 2 (16) the TTT molecule is the same as reported by Smith and Luss (Kodak) (9) and very similar to neutral TTT (17). In general there are no features in this room temperature structure which might suggest that there is any significant difference in the TTT framework between the TTT_2I_3 crystals from JPL and those from Kodak. From the description given by Buravov, et al., (Chernogolovka) (6) their TTT_2I_3 crystals also have the same framework. Mihály, Jańossy, and Grüner (Budapest) did not report any structural data but apparently believe that their TTT_2I_3 crystals have the same structure as the Kodak and Chernogolovka crystals (18). However, the physical properties of TTT_2I_3 crystals are dependent on which laboratory grew the crystals. This suggests that variations in the properties of TTT_2I_3 may arise from variations in the iodide channels.

Shown in Figure 3 is the electron density of the iodide channels based on the refinement of the TTT lattice. Shown in Figure 4 are the corresponding difference Fourier sections which indicate that a

Table III

TTT Geometry in TTT_2I_3 (h.d.) ~294° K (CuK_α)

Bond Lengths, Å*		Interior Bond Angles*	
C1-C1	1.422(10)	C1-C1-C2	119.6(8)°
C3-C3	1.455(8)	C1-C2-S	114.1(3)
C5-C5	1.438(10)	C2-S-S	95.5(2)
C1-C2	1.387(7)	C2-C1-C2	120.8(8)
C2-C3	1.413(6)	C1-C2-C3	122.2(4)
C3-C4	1.412(6)	C2-C3-C3	118.2(7)
C4-C5	1.349(7)	C3-C3-C4	118.2(7)
S-C2	1.746(4)	C3-C4-C5	121.7(4)
S-S	2.080(2)	C4-C5-C5	120.1(8)
H1-C4	1.01(6)	H1-C4-C3	113(3)
H2-C5	1.07(5)	H1-C4-C5	125(3)
		H2-C5-C4	121(3)
		H2-C5-C5	119(3)

Direction cosines of the plane normal 0.0, -0.6700, 0.7424 (best plane calculation of inner carbon rings).

TTT tilt angle to $\vec{b}$ 47.93°.

Interplanar spacing 3.324 Å (b = 4.962 Å).

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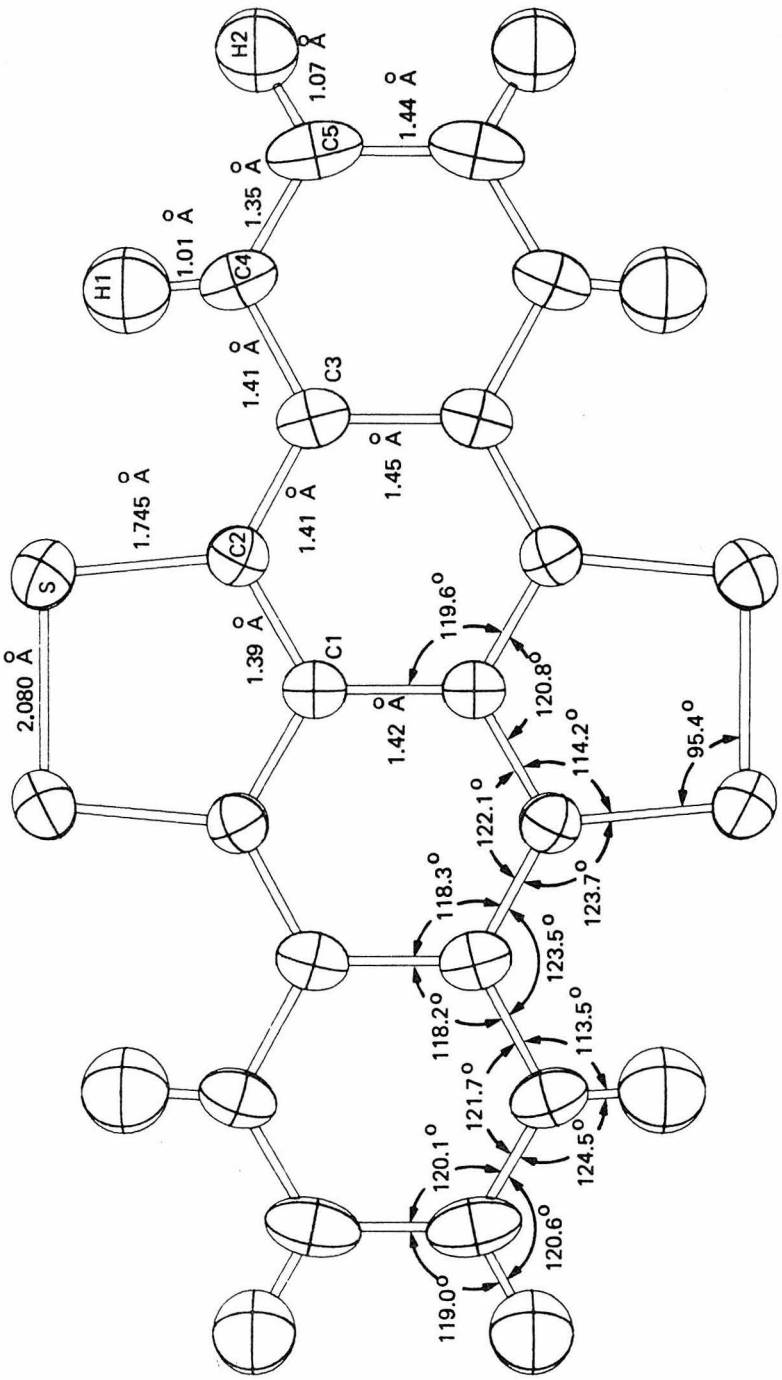
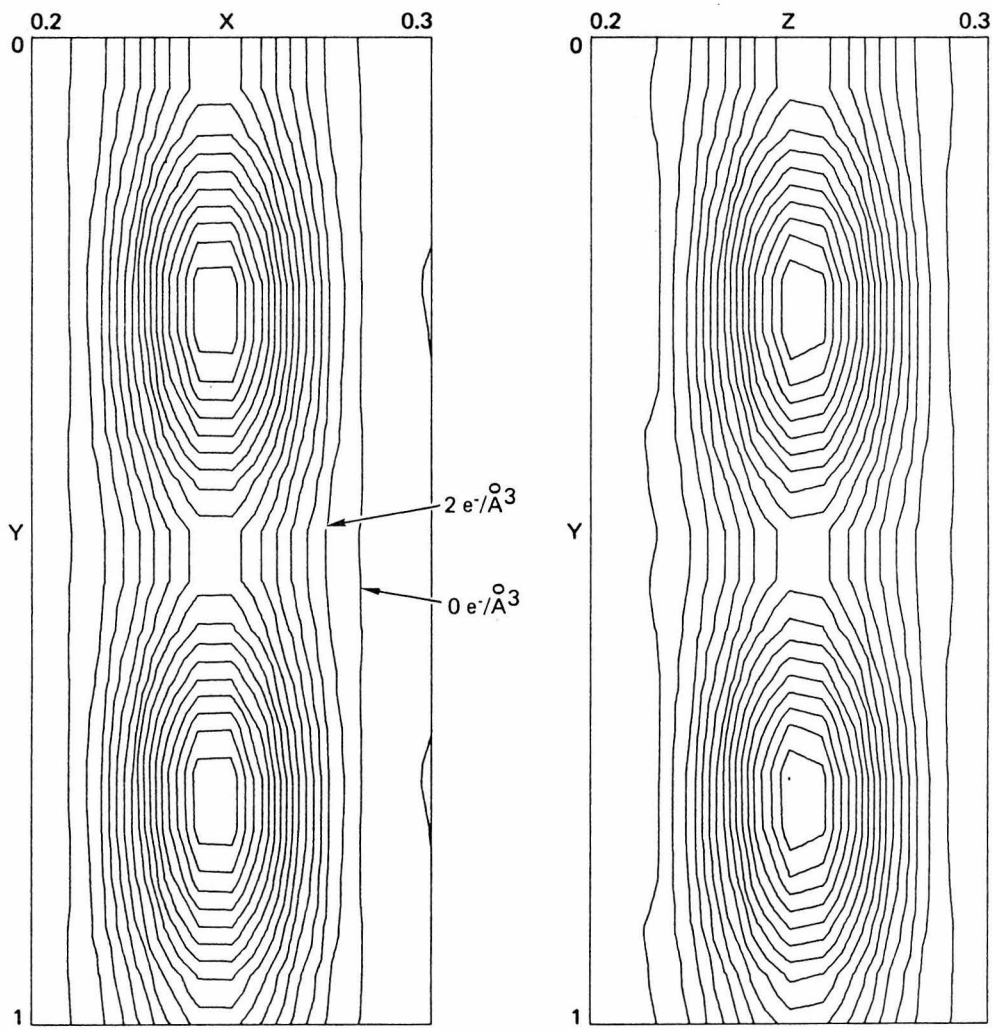
*The deviation in the last decimal place is given in parentheses (assuming isotropic atoms).



Tetrathiotetracene cation in high disorder TTT_2I_3 at room temperature
Thermal ellipsoids are drawn at the 50% probability level

Figure 2

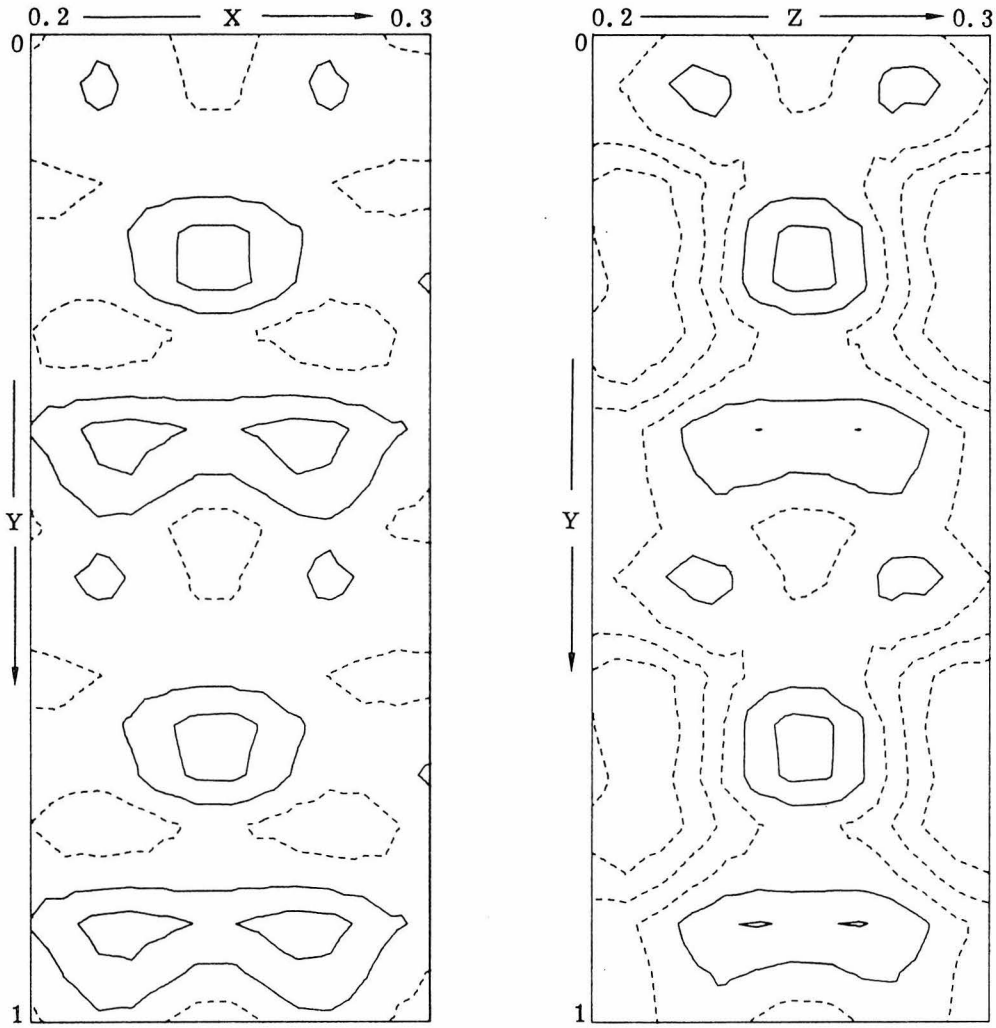


TTT_2I_3 (h.d.) - Room Temperature

Electron Density Along Iodine Channel

Contoured at 2 electrons/Å^3 Intervals

Figure 3



TTT_2I_3 (h.d.) - Room temperature
Difference Fourier Sections through Iodine Channel
Contoured at 0.2 electrons /$\mathring{A}^3$ Intervals
-------- negative contours
———— zero and positive contours

Figure 4

reasonable fit has been obtained for the observed and calculated electron density. Figure 3 shows that there are not discrete iodide sites in a spacing of b = 4.96 Å. The two broad maxima are related by symmetry and are only 4.96 Å/2 = 2.48 Å apart. This distance is too short for any chemically reasonable iodide species. That there is also significant electron density at the minima, suggests that Figure 3 represents an average of, perhaps, several iodide configurations present in different channels throughout the structure. This could be caused by slippage of the iodide chains parallel to $\vec{b}$. The minimum and maximum are 12.9 $e^-/Å^3$ and 32.9 $e^-/Å^3$ respectively. The refined population, the only iodine parameter from Table II of any significance, gives a stoichiometry of $TTTI_{1.41\pm.08}$. The Kodak crystals exhibit minima and maxima of 16 $e^-/Å^3$ and 37 $e^-/Å^3$ for a refinement based on a stoichiometry of $TTTI_{1.5}$. (The iodine population was not refined.) The difference in the maximum and minimum electron densities between TTT_2I_3 (h.d.) and the Kodak crystals could be due to different size grids in the Fourier maps. The similarities between the structural and photographic data reported for Kodak crystals (9) and the data obtained for TTT_2I_3 (h.d.) suggest that the physical properties of crystals from Kodak and JPL ought to be similar, as, in fact, they are (10). It is unfortunate that there is no detailed structural information available for the Chernogolovka or Budapest crystals for comparison with the Kodak and JPL crystals. Detailed information about the Chernogolovka crystals would be especially interesting because those crystals have different properties from those of JPL or Kodak.

2.2 Low-Temperature Structures

Experimental

For the low-temperature studies a new, locally designed and built, goniometer was used. The goniometer is used on a modified, full-circle Syntex $P\bar{1}$ automated diffractometer. The outer shell of the goniometer is a sphere which has kaptan-sealed entrance and exit slits for the X-rays. The volume enclosed by the sphere is evacuated. Inside the crystal is enclosed by two additional,cooled, inner shells. The innermost copper shell surrounding the crystal is attached directly, mechanically and thermally, to the extended tip of the cryocooler (extender). The cryocooler is a Cryogenics Technology Inc. closed-cycle helium gas refrigerator rated to cool to ~10°-14° K. The crystal is cooled by a copper heat-transfer cable which thermally links the top of the phi-shaft to the cold, inner shell (19).

The crystal of TTT_2I_3 (h.d.) used for data collection, the fifth one of six studied, was a six-sided needle 0.333 mm long and had a cross-sectional area of 0.00686 mm^2. The crystal was mounted on a glass fiber with Armstrong low-temperature epoxy resin. The glass fiber was mounted onto a copper pin which was inserted directly into the copper block at the top of the phi-shaft. Crystal alignment was accomplished by bending the copper pin. At room temperature the crystal was set high, above the center of the diffractometer, to allow for shrinkage at low temperatures. Temperatures were continuously

monitored at the extender (extended tip of the cryocooler) and just underneath the copper pin at the top of the phi-shaft. The temperature of the innermost copper shell could also be measured. At temperatures between 18.5° and 25.5° K the diode measuring the phi-shaft temperature gave correct, accurate readings. Between 26.5° K and liquid N_2 (77.4° K) the diode gave low readings, the largest correction being +4.7° at 35.5° K. No calibration was done at higher temperatures. Unless otherwise stated, the temperatures reported are the observed uncorrected temperatures at the phi-shaft. The rate at which the crystal was cooled could be controlled by how often the temperature at the extender was lowered. From room temperature (~294° K) to ~164° K the fifth crystal was cooled at 10° per 30-60 minutes in 2° steps. After every 10° the crystal was equilibrated for one to twelve hours while peak intensities and scans of several reflections were obtained.

At 164° K a data set was collected with monochromatized molybdenum K_α radiation. The unit cell parameters listed in Table IV were obtained from a constrained least-squares fit of the 2θ values for thirty computer-centered reflections (20). The symmetry during the least-squares fit was constrained to be orthorhombic. Intensities of the TTT lattice reflections were collected with 1° per minute 2θ-θ scans. Total time of background counting was 25% of the amount of time spent scanning a reflection. Backgrounds were collected on each side of a reflection. The observed range of temperatures at the

Table IV

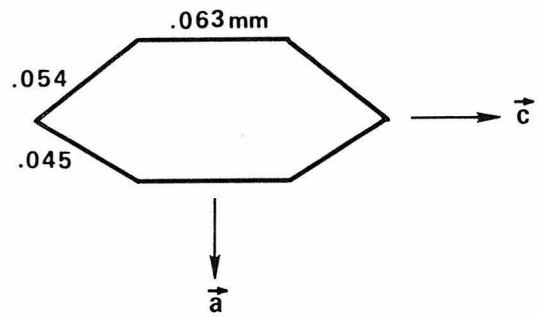
Crystal Data for TTT_2I_3 (h.d.)

Orthorhombic, Space group Cmca

Z = 2

Linear absorption coefficient (MoK_α), μ = 33.5225 cm^{-1}.

Crystal dimensions: length 0.333 mm
cross-sectional area 0.00686 mm^2



	~164° K	~74° K	~19° K
a =	18.285(3) Å	18.246(4) Å	18.225(3) Å
b =	4.957(1)	4.947(1)	4.950(1)
c =	18.351(3)	18.284(5)	18.242(6)
V =	1663(1) $Å^3$	1650(1) $Å^3$	1646(1) $Å^3$

($MoK_{\overline{\alpha}}$, λ = 0.71069 Å)

phi-shaft during data collection was 163.7° and 167° K. The temperature at the extender varied by ±0.1°.

After 366 hours of data collection cooling was resumed. The rate of cooling was 10°/hour in 1° steps with peak scans every ten degrees. Below about 90° K the crystal was cooled at 5°/hour in 0.5° steps with peak scans every ten degrees to ~74° K. At 74° K a data set was again collected with monochromatized molybdenum K_α radiation. The unit cell parameters listed in Table IV were obtained from a symmetry-constrained least-squares fit of the 2θ values of twenty-nine computer-centered reflections (20). Intensities were collected as at 164° with 1° per minute 2θ-θ scans. The total time for background counting was 20% of the amount of time for each scan at low angle and 30% at high 2θ values. The background counting time was changed during the data collection if the scan width was also changed. The percentage was chosen so that the background on each side of a reflection was collected for 25-45 seconds. A shell of data for a primitive cell was collected to check that the centering condition had not changed. No violations were observed. During the data collection the average temperature at the phi-shaft was about 73°-74° K with a total range of about three degrees. The innermost cold shell surrounding the crystal was at 62.7° K.

After 377 hours of data collection, cooling was resumed. The temperature was lowered at 0.1° per minute with equilibration and peak scans every ten degrees until the lowest temperature, 20° K, was reached. During the first fifty-five hours of data collection the phi-shaft temperature gradually dropped from ~20° K to 18.9° K at which

point the heater was turned on to prevent any further temperature drop. During the remainder of the data collection the temperature at the phi-shift remained between 18.6° and 19.6° K. Intensities were collected as before with 1° per minute 2θ-θ scans. Total time for background counting was 25% of the scan time per reflection for low-angle reflections and 35% at high angles. Part of the data was collected for a primitive cell to check for violations of the lattice centering. In addition to the complete data set obtained for the octant $\bar{h}k\ell$, part of octants $\overline{h}\overline{k}\ell$ and $hk\ell$ were also collected to check if the lattice symmetry had changed. No violations of the orthorhombic lattice symmetry or of the C-centering were observed. Towards the end of the data collection a slight decay of about 2% in the intensities of the check reflections was observed. The unit cell parameters listed in Table IV were obtained from a symmetry-constrained least-squares fit of twenty-two computer-centered reflections (20).

The integrated intensities for all three sets of data of the TTT lattice were corrected for Lorentz and polarization effects and for absorption (μ = 33.5225 cm^{-1}) (12,13). No correction was made for the slight decay observed towards the end of the data set collected at 19° K. The weights used in refinement were based on counting statistics. No more than two observations contributed to a weight. The F_o for reflections with more than one observation is a weighted average of the F^2 values (21). No reflections were observed at 164° K 74° K, or 19° K which would violate the space group Cmca.

Initial atomic coordinates for the structure at 164° K were obtained from a three-dimensional Patterson map. Successive iterations of structure factor calculations followed by Fourier synthesis were used until all the atomic coordinates, except for the hydrogen atoms, were known. The real part ($f_0 + \Delta f'$) of the atomic scattering factor corrected for anomalous dispersion was used for iodine and sulfur for the structures at all three temperatures (14). As at room temperature two iodine atoms were used to fit the electron density in the channels at 1/4, y, 1/4. Their positions were determined from difference Fourier sections. All of the structural parameters, except the iodine coordinates, were refined by the full-matrix least-squares method. After the structure was partially refined, the hydrogen atoms were observed on a three-dimensional difference Fourier map. The hydrogen parameters were included in the final least-square cycles. The refinement converged to R = 0.082, with a goodness-of-fit = 1.42 for the complete data set of 1338 reflections of which 1160 reflections had F_o^2 greater than zero (15). For the 731 reflections with $F_o^2 \geq 3\sigma(F_o^2)$, R = 0.042.

The carbon and sulfur atomic coordinates from the 164° K structure were used as input to the initial structure factor calculations for the 74° K structure. The iodine atomic coordinates were determined from Fourier and difference Fourier sections. After preliminary refinement the hydrogen atoms were located on a low-angle difference Fourier map. Full-matrix least-squares refinement was used to refine all of the structural parameters except for the iodine coordinates. The structure

in space group Cmca converged to R = 0.081, with a goodness-of-fit = 1.42 for a complete data set of 1670 reflections of which 1506 had F^2 greater than zero. For the 982 reflections with $F_o^2 \geq 3\sigma(F_o^2)$, R = 0.042.

Because there were no observed violations of the systematic absences for the space group Cmca or any indications for a change in lattice symmetry, initial structure factor calculations for the structure at 19° K were based on the sulfur and inner-ring carbon atom coordinates at 74° K. The atomic coordinates were gradually added through successive iterations of structure factor-Fourier calculations. The data set at 19° K had h0ℓ reflections to 2θ = 108° and hkℓ, k > 0 reflections to 2θ = 70°, so a low-angle cut-off of the data was used during the early phase of structure determination. The electron density in the channel could still be fit reasonably well with two iodine atoms representing the broad maximum. For the final full matrix least-squares refinement the complete data set was used. For the space group Cmca the refinement converged to R = 0.073, with the goodness-of-fit = 1.35 for the complete data set of 1984 reflections, of which 1792 reflections had F_o^2 greater than zero. For the 1194 reflections which had $F_o^2 \geq 3\sigma(F_o^2)$, R = 0.039.

Listed in Tables V, VI, and VII are the atomic coordinates and thermal parameters. The bond lengths and bond angles for the refined structures at 164° K, 74° K, and 19° K are listed in Tables VIII, IX, and X. Complete lists of the observed and calculated structure factors are in Appendix C.

Table V

Atomic Coordinates and Thermal Parameters for TTT_2I_3 (h.d.) at ~164° K (MoK_α)

	X	Y	Z	Populations
I1	.25	.325	.25	1.1335(183)
I2	.25	.182	.25	.4655(180)
C1	.03904(21)	0	0	
C2	.07679(15)	.18186(58)	.04458(16)	
C3	.03948(16)	.36770(63)	.08940(15)	
C4	.07619(20)	.55735(67)	.13443(17)	
C5	.03876(19)	.73805(75)	.17622(17)	
S	.17154(5)	.15337(18)	.03883(5)	

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I1	.0240(7)	.3519(52)	.0319(7)	0	-.0050(5)	0
I2	.0332(27)	.2022(149)	.0367(25)	0	.0239(16)	0
C1	.0136(19)	.0136(21)	.0148(17)	0	0	.0025(20)
C2	.0134(13)	.0143(15)	.0190(12)	-.0024(15)	-.0011(11)	.0045(15)
C3	.0209(15)	.0142(14)	.0151(12)	-.0017(16)	-.0007(11)	.0034(15)
C4	.0249(17)	.0188(17)	.0169(13)	-.0037(18)	-.0056(13)	.0036(14)
C5	.0431(22)	.0196(16)	.0134(12)	-.0033(18)	-.0055(14)	-.0009(15)
S	.0151(4)	.0235(4)	.0325(4)	-.0020(5)	-.0021(4)	-.0051(4)

	X	Y	Z	B
H1	.1298(17)	.5594(61)	.1333(16)	1.52(0.71)
H2	.0667(18)	.8703(66)	.2064(18)	2.11(0.77)

Table VI

Atomic Coordinates and Thermal Parameters for TTT_2I_3 (h.d.) at ~74° K (MoK_α)

	X	Y	Z	Populations
I1	.25	.328	.25	1.1230(138)
I2	.25	.189	.25	.3757(135)
C1	.03913(18)	0	0	
C2	.07685(12)	.18273(53)	.04472(13)	
C3	.03972(13)	.36936(55)	.08954(12)	
C4	.07657(15)	.56009(58)	.13460(13)	
C5	.03894(15)	.74221(65)	.17640(12)	
S	.17211(4)	.15388(15)	.03901(3)	

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I1	.0125(5)	.3318(39)	.0162(4)	0	-.0032(4)	0
I2	.0148(17)	.1879(105)	.0159(12)	0	.0128(9)	0
C1	.0086(14)	.0107(17)	.0095(11)	0	0	.0015(14)
C2	.0091(10)	.0096(12)	.0122(8)	-.0009(12)	-.0012(8)	.0022(10)
C3	.0120(10)	.0093(12)	.0104(8)	.0000(12)	-.0015(8)	.0027(10)
C4	.0152(12)	.0130(14)	.0111(8)	-.0011(14)	-.0018(9)	.0014(10)
C5	.0247(14)	.0106(12)	.0105(8)	-.0018(14)	-.0029(9)	.0006(11)
S	.0092(3)	.0131(3)	.0200(3)	-.0011(4)	-.0011(2)	-.0029(3)

	X	Y	Z	B
H2	.0671(15)	.8734(59)	.2085(14)	.73(0.58)
H1	.1297(15)	.5595(57)	.1326(14)	.72(0.59)

Table VII

Atomic Coordinates and Thermal Parameters for TTT_2I_3 (h.d.) at ~19° K (MoK_α)

	X	Y	Z	Populations
I1	.25	.329	.25	1.014(211)
I2	.25	.201	.25	.4916(211)
C1	.03937(15)	0	0	
C2	.07700(10)	.18251(44)	.04485(12)	
C3	.03965(11)	.37076(48)	.08976(11)	
C4	.07696(12)	.56103(51)	.13477(12)	
C5	.03897(13)	.74358(57)	.17650(11)	
S	.17235(3)	.15438(13)	.03909(3)	

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I1	.0045(3)	.3132(63)	.0072(4)	0	-.0013(3)	0
I2	.0115(10)	.2624(132)	.0081(9)	0	.0054(6)	0
C1	.0068(9)	.0085(13)	.0066(9)	0	0	.0003(12)
C2	.0073(7)	.0066(9)	.0089(7)	.0002(9)	-.0006(6)	.0020(8)
C3	.0078(6)	.0074(9)	.0076(6)	.0014(9)	-.0001(6)	.0018(8)
C4	.0110(8)	.0107(10)	.0084(7)	-.0010(10)	-.0026(6)	.0005(8)
C5	.0174(9)	.0099(9)	.0064(7)	.0002(11)	-.0020(7)	.0006(9)
S	.0066(2)	.0093(2)	.0149(2)	-.0005(3)	-.0012(2)	-.0022(3)

	X	Y	Z	B
H1	.1281(17)	.5641(61)	.1322(17)	1.58(0.68)
H2	.0672(17)	.8788(65)	.2088(18)	1.75(0.70)

Table VIII

TTT Geometry in TTT_2I_3 (h.d.) ~164° K (MoK_α)

Bond Lengths, Å*		Interior Bond Angles*	
C1-C1	1.428(8)	C1-C1-C2	119.5(6)°
C3-C3	1.444(6)	C1-C2-S	113.8(2)
C5-C5	1.417(7)	C2-S-S	95.8(2)
C1-C2	1.399(5)	C2-C1-C2	120.9(6)
C2-C3	1.411(4)	C1-C2-C3	121.5(3)
C3-C4	1.420(4)	C2-C3-C3	118.9(6)
C4-C5	1.363(5)	C3-C3-C4	118.2(6)
S-C2	1.742(3)	C3-C4-C5	121.7(3)
S-S	2.084(2)	C4-C5-C5	120.1(6)
H1-C4	0.98(3)	H1-C4-C3	118(2)
H2-C5	0.999(33)	H1-C4-C5	120(2)
		H2-C5-C4	119(2)
		H2-C5-C5	121(2)

Direction cosines of the plane normal 0.0, -0.6690, 0.7433 (Best plane calculation of inner carbon rings).

TTT tilt angle to $\vec{b}$ 48.02°.

Interplanar spacing 3.316 Å.

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*The standard deviations in the last decimal place are given in parentheses (assuming isotropic atoms).

Table IX

TTT Geometry in TTT_2I_3 (h.d.) ~74° K (MoK_α)

Bond Lengths, Å*		Internal Bond Angles*	
C1-C1	1.428(7)	C1-C1-C2	119.5(6)°
C3-C3	1.449(5)	C1-C2-S	113.7(2)
C5-C5	1.421(6)	C2-S-S	95.8(1)
C1-C2	1.400(4)	C2-C1-C2	121.1(5)
C2-C3	1.408(3)	C1-C2-C3	121.8(2)
C3-C4	1.422(4)	C2-C3-C3	118.8(4)
C4-C5	1.367(4)	C3-C4-C5	121.6(2)
S-C2	1.747(5)	C4-C5-C5	120.2(5)
S-S	2.087(1)	H1-C4-C3	117(2)
H1-C4	0.97(3)	H1-C4-C5	122(2)
H2-C5	1.01(3)	H2-C5-C4	119(2)
		H2-C5-C5	120(2)

Direction cosines of the plane normal 0.0, -0.6673, 0.7448 (best plane calculation of inner carbon rings).

TTT tilt angle to $\vec{b}$ 48.14°.

Interplanar spacing 3.301 Å.

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*The deviations in the last decimal place are given in parentheses (assuming isotropic atoms).

Table X

TTT Geometry in TTT_2I_3 (h.d.) ~19° K (MoK_α)

Bond Lengths, Å*		Internal Bond Angles*	
C1-C1	1.435(6)	C1-C1-C2	119.4(5)°
C3-C3	1.445(4)	C1-C2-S	113.7(2)
C5-C5	1.420(5)	C2-S-S	95.7(1)
C1-C2	1.399(3)	C2-C1-C2	121.3(4)
C2-C3	1.415(3)	C1-C2-C3	121.9(2)
C3-C4	1.423(3)	C2-C3-C3	118.7(4)
C4-C5	1.369(3)	C3-C4-C5	121.1(2)
S-C2	1.747(2)	C4-C5-C5	120.4(4)
S-S	2.090(1)	H1-C4-C3	117(2)
H1-C4	0.93(3)	H1-C4-C5	121(2)
H2-C5	1.03(3)	H2-C5-C4	120(2)
		H2-C5-C5	120(2)

Direction cosines of the plane normal 0.0, -0.6657, 0.7462 (best plane calculation of inner carbon rings).

TTT tilt angle to $\vec{b}$ 48.26°.

Interplanar spacing 3.295 Å.

---

*The deviations in the last decimal place are given in parentheses (assuming isotropic atoms).

Discussion

ORTEP drawings (16) of the TTT molecule at 164° K, 74° K, and 19° K are shown in Figures 5, 6, and 7. There is nothing unusual with the geometry of the TTT molecules. Table XI lists, for comparison, the bond lengths of neutral TTT (17), the bond lengths of TTT in Kodak's TTT_2I_3, and the bond lengths as a function of temperature for TTT_2I_3 (h.d.). The geometry of TTT in all of the structures is very similar. The S-S bond seems to lengthen with decreasing temperature. The orientation of adjacent TTT molecules in the same stack remains about the same at 19° K as at room temperature (Figure 8). The angle of the TTT tilt to the b axis increases slightly with decreasing temperature. The interplanar distance between TTT molecules decreases as the temperature is lowered (Tables VIII, IX, X).

A comparison of Figure 3 with Figure 9 indicates that, except for a loss of thermal motion perpendicular to the channel and a general increase in coherently scattering electron density, the channel structure remains the same at 164° K as at room temperature (~294° K). At 294° K the maximum and minimum electron density in the channel are 12.9 e/Å^3 and 32.9 e/Å^3. At 164° K the minimum and maximum are 26.9 e/Å^3 and 58.4 e/Å^3. Although the amount of coherently scattering electron density in the channel continues to increase with decreasing temperature, the channel structure at 19° K is essentially the same as at room temperature (Figures 11 and 13). The position of the broad maximum does shift a little (Table XII). Figures 10, 12, and 14 are the

Table XI

Comparison of TTT Molecular Geometry

	TTT[a]	TTT_2I_3[b]	TTT_2I_3 (h.d.)[c]	TTT_2I_3 (h.d.)[d] 164° K	74° K	19° K
C1-C1	1.42(1)	1.429(8)	1.422(10)	1.428(8)	1.428(7)	1.435(6)
C1-C2	1.41(1)	1.390(4)	1.387(6)	1.399(5)	1.400(4)	1.398(4)
C2-C3	1.37(1)	1.414(4)	1.413(6)	1.411(4)	1.408(3)	1.415(3)
C3-C3	1.46(1)	1.444(6)	1.455(8)	1.444(6)	1.449(5)	1.445(4)
C3-C4	1.45(1)	1.410(5)	1.412(6)	1.420(4)	1.422(4)	1.423(3)
C4-C5	1.37(1)	1.358(5)	1.350(7)	1.363(5)	1.367(4)	1.369(3)
C5-C5	1.42(1)	1.404(8)	1.438(10)	1.417(7)	1.421(6)	1.420(4)
C2-S	1.78(1)	1.738(3)	1.746(4)	1.742(3)	1.747(3)	1.747(2)
S-S	2.100(3)	2.078(2)	2.080(2)	2.084(2)	2.086(1)	2.090(1)
inter-planar spacing[e]		3.32(2)	3.324(2)	3.316(2)	3.301(2)	3.295(2)

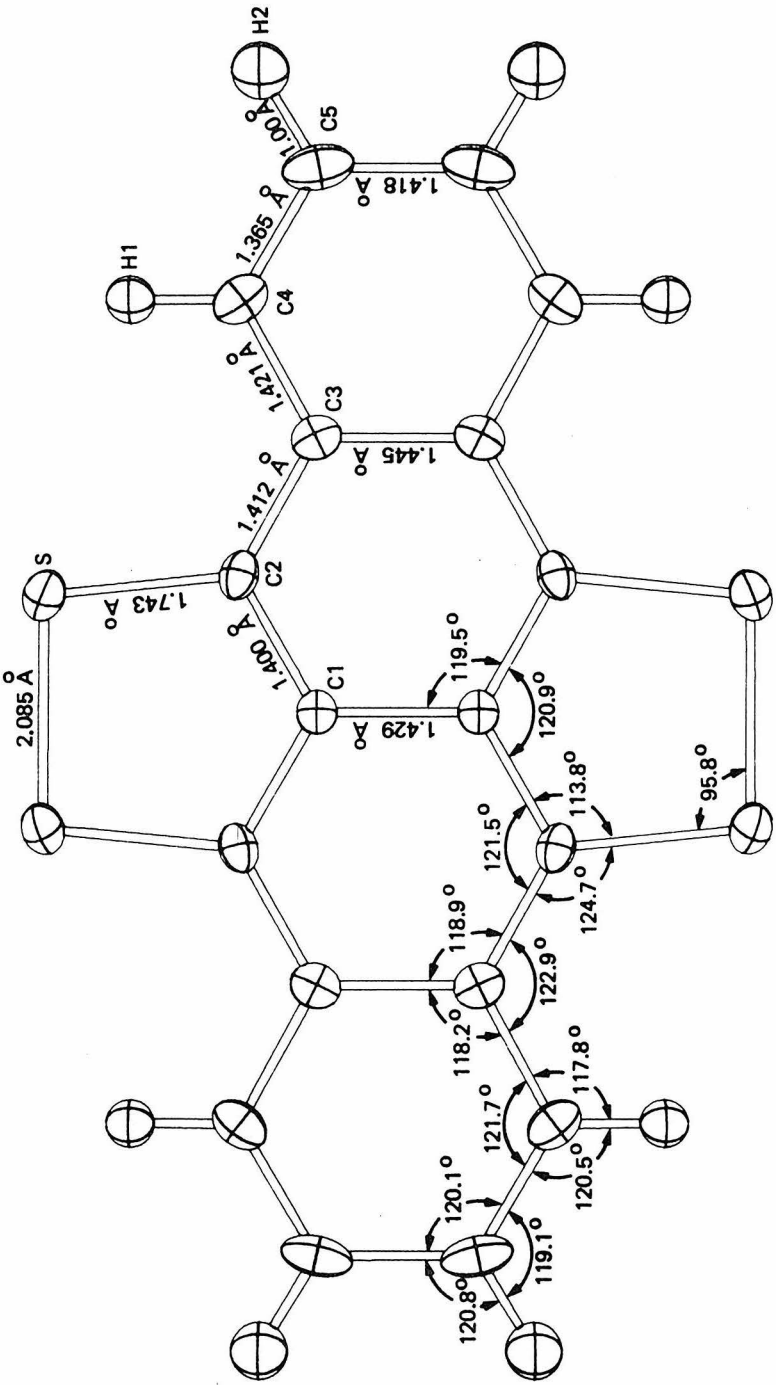
[a]Dideberg and Toussaint (1974) (17), CuK_α, room temperature. Neutral TTT crystallizes in space group $P\bar{1}$: the bond lengths in this table are an average of the values reported by Dideberg and Toussaint.

[b]Smith and Luss (1977) (9), MoK_α, room temperature.

[c]This study, CuK_α, room temperature.

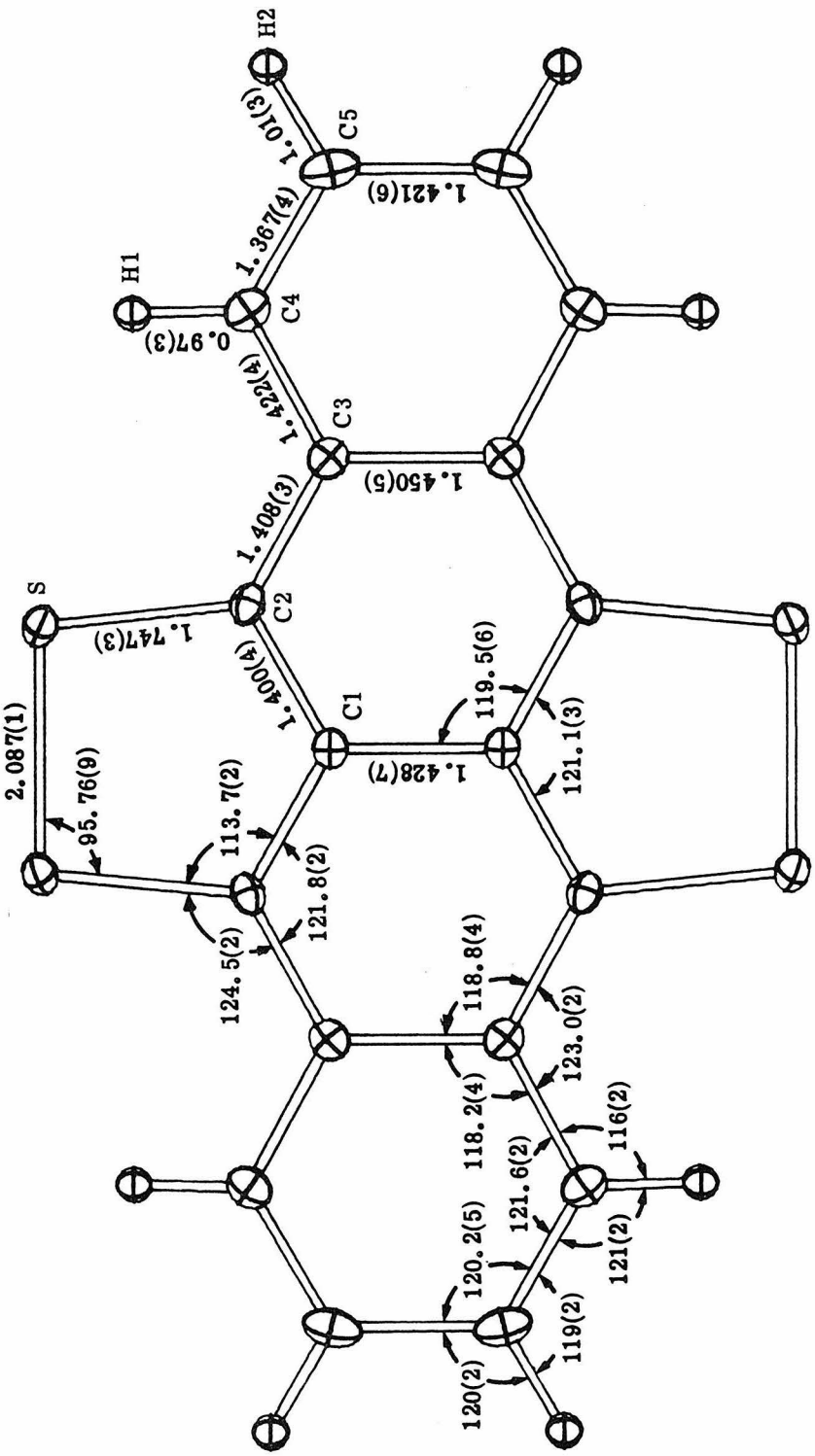
[d]This study, MoK_α, sigmas are for isotropic atoms and neglecting unit cell errors.

[e]The interplanar spacing reported for this study are based on the best least-squares plane of just the inner TTT rings (C_1 C_2 C_3).



Tetrathiotetracene cation in high disorder TTT_2I_3 at 164°K.
Thermal ellipsoids are drawn at the 50% probability level

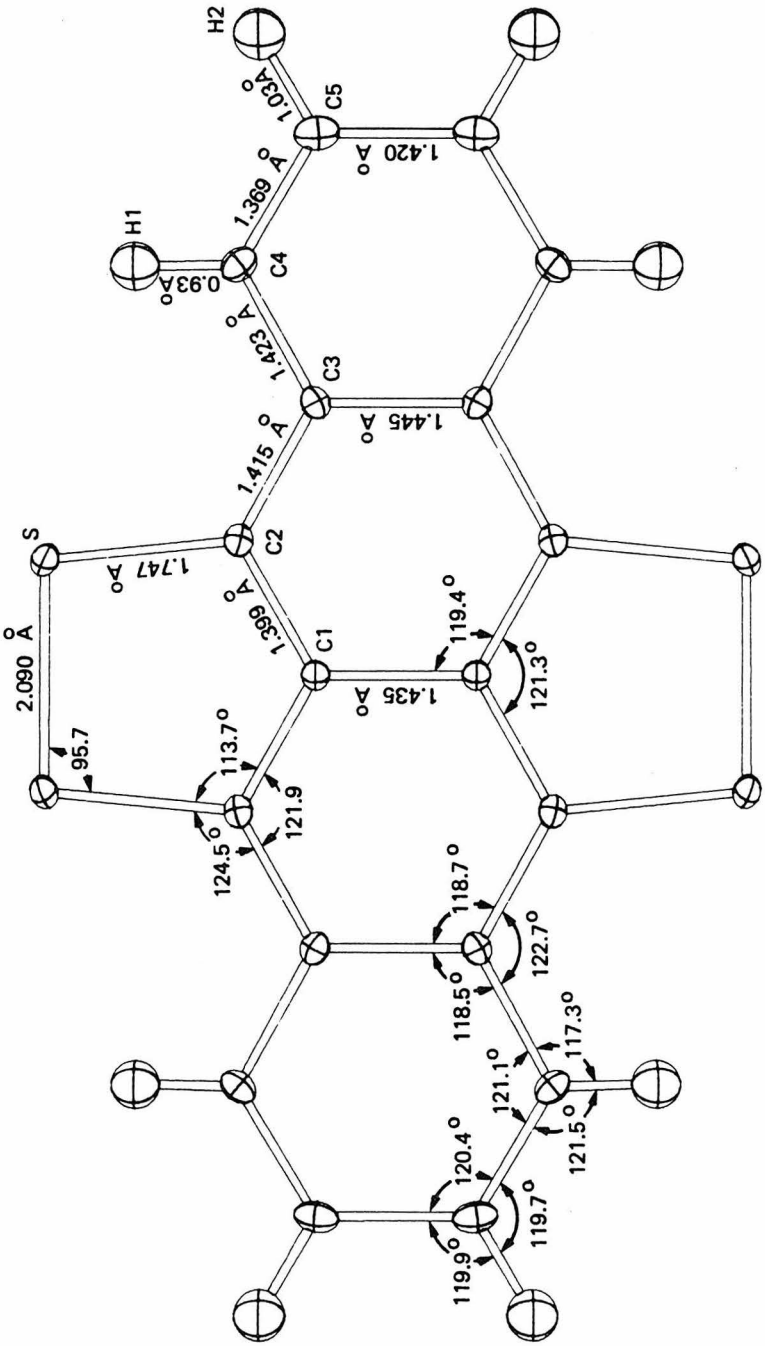
Figure 5



Tetrathiotetracene Cation in TTT_2I_3(h.d.) at 74 °K

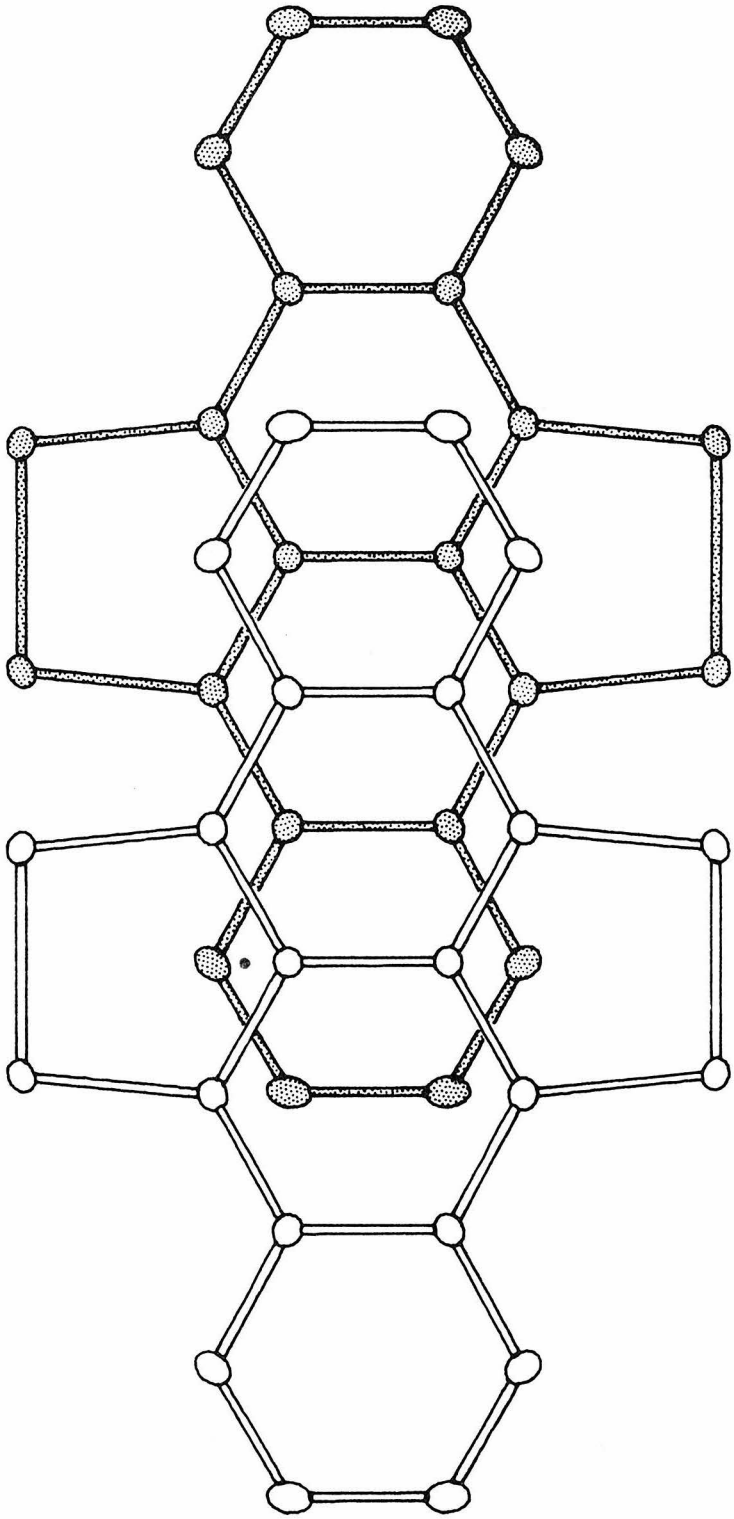
Thermal ellipsoids are drawn at the 50% level.

Figure 6



Tetrathiotetracene cation in high disorder TTT_2I_3 at 19°K.
Thermal ellipsoids are drawn at the 50% probability level

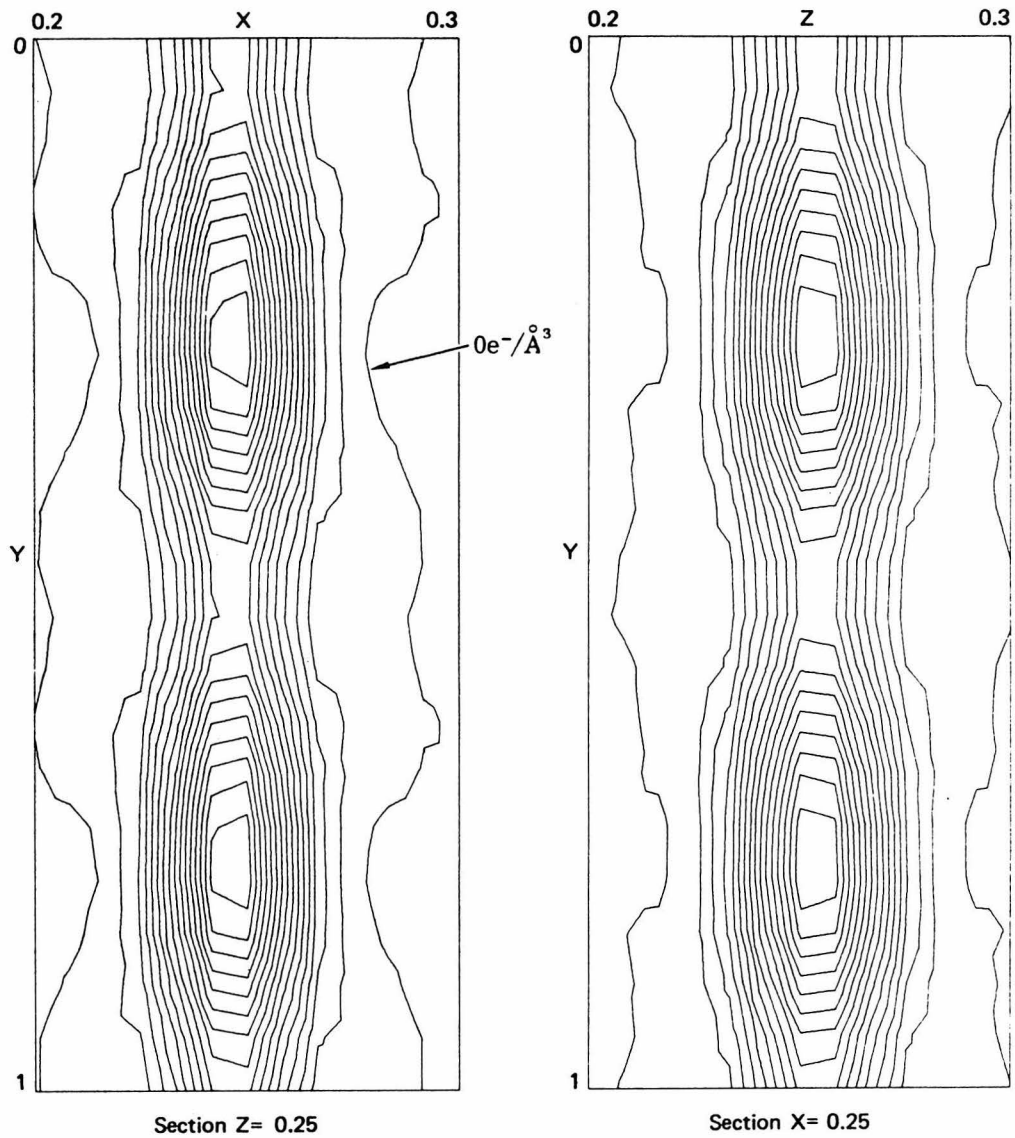
Figure 7



Neighboring tetrathiotetracene molecules in the same cation stack

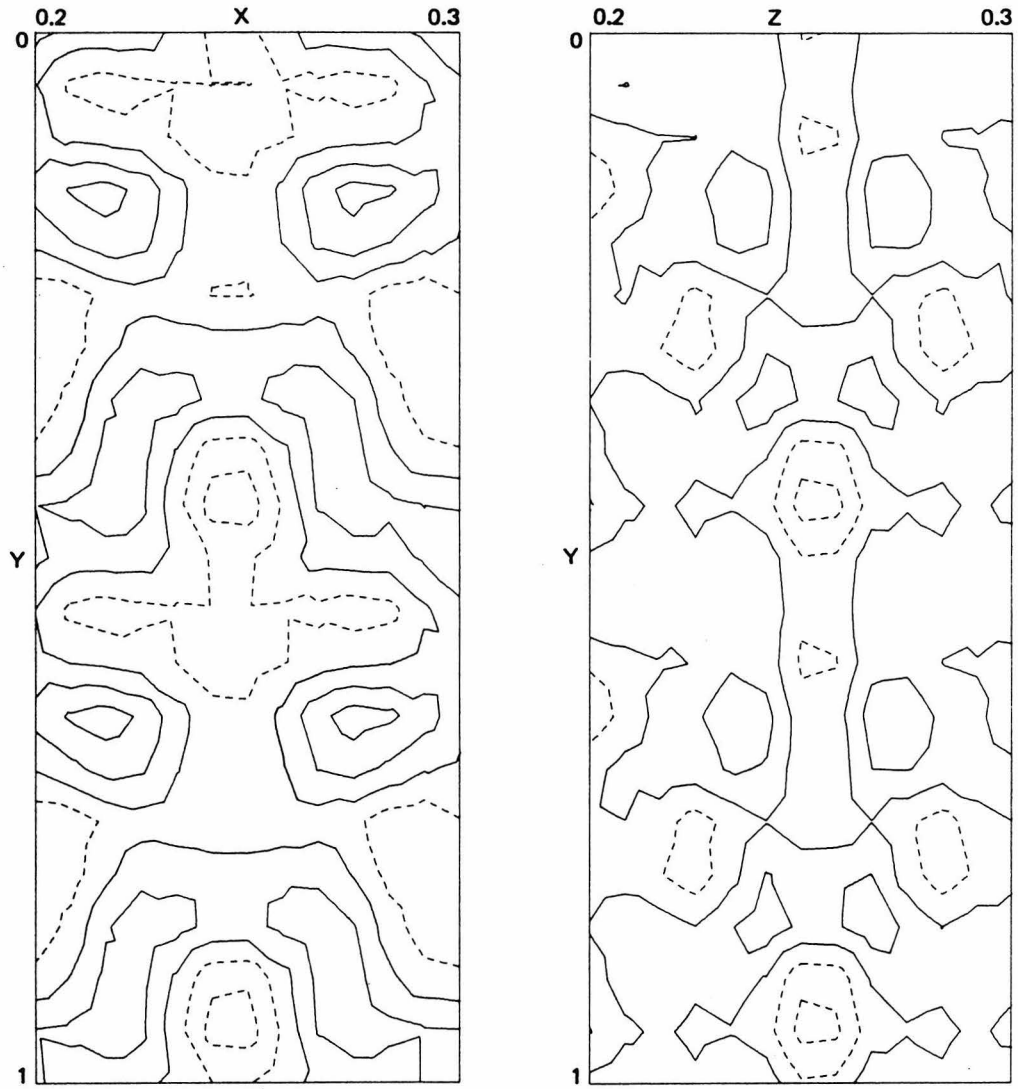
TTT_2I_3 (h.d.) $\phi \sim 19°K$

Figure 8



TTT_2I_3 (h.d.) at 164°K
Electron Density along Iodine Channel
Contoured at 3.5 electrons/Å^3 intervals beginning at zero

Figure 9



TTT_2I_3 (h.d.) at 164°K

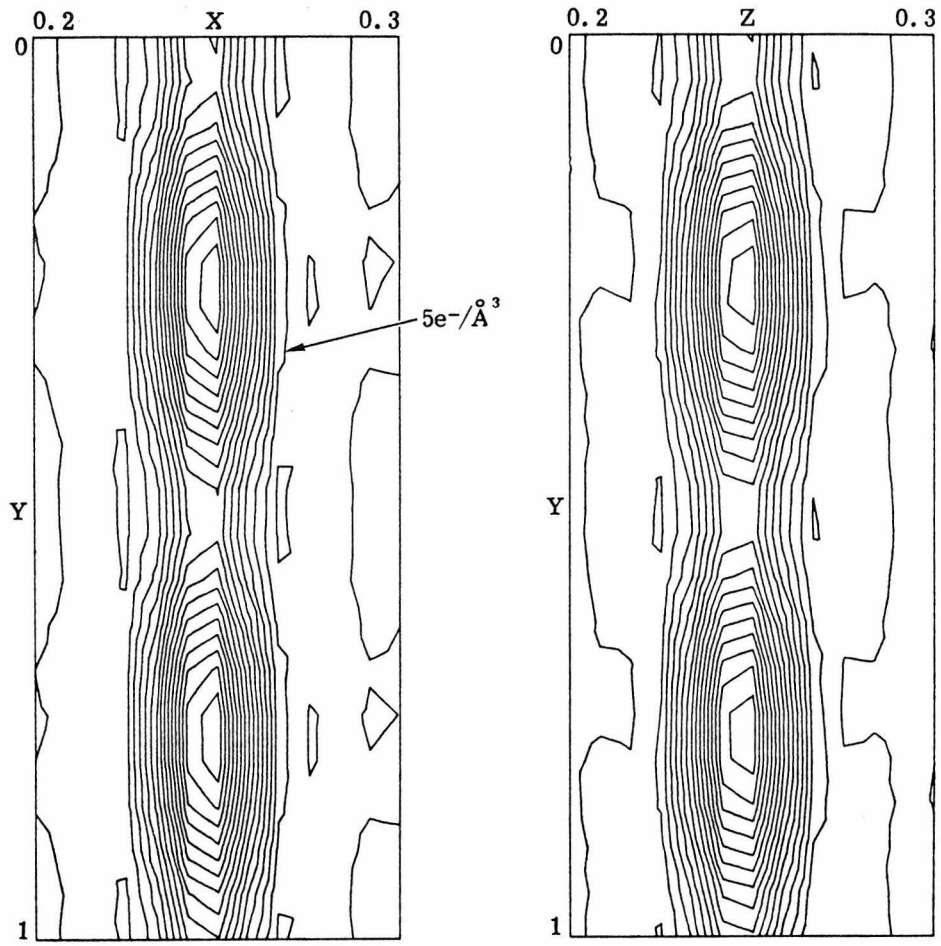
Difference Fourier Sections through Iodine channel

Contoured at 0.5 electrons / A^3 interval

– – – – – – – negative contours

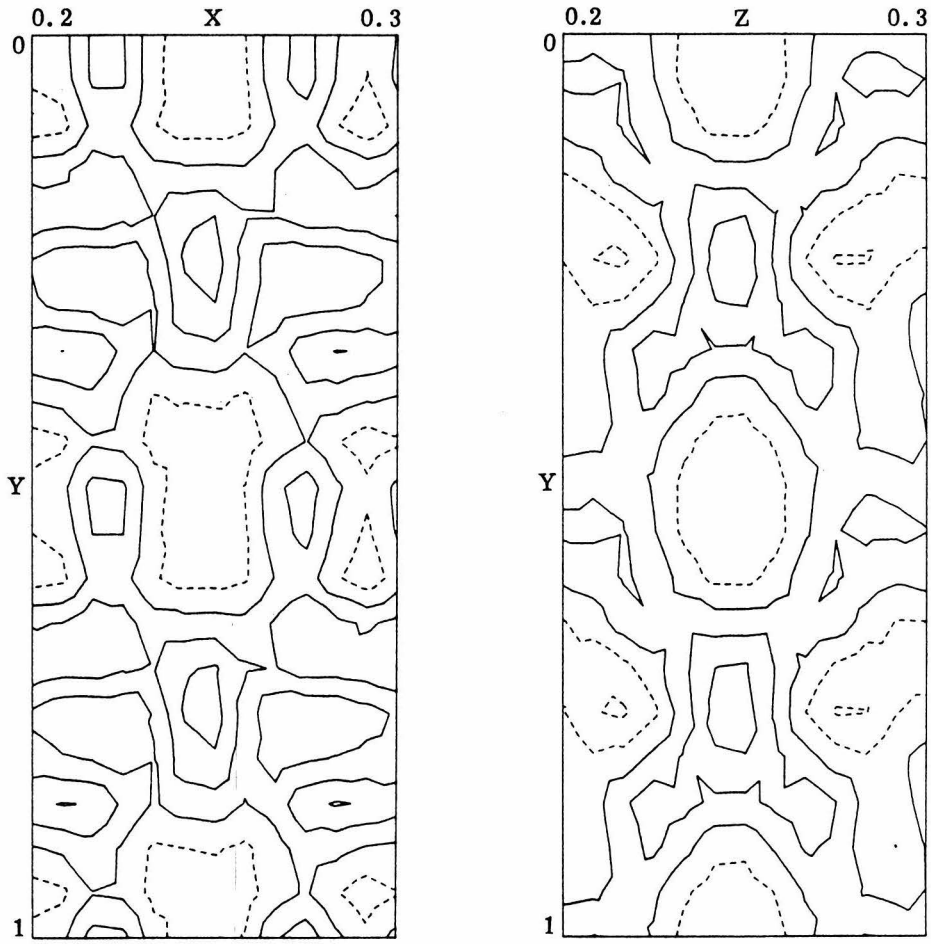
——————— zero and positive contours

Figure 10



TTT_2I_3 (h.d.) at 74°K
Electron Density along Iodine Channel
Contoured at 5 electrons/Å^3 intervals beginning at zero

Figure 11



Section Z= 0.25 Section X= 0.25

TTT_2I_3 (h.d.) at 74°K

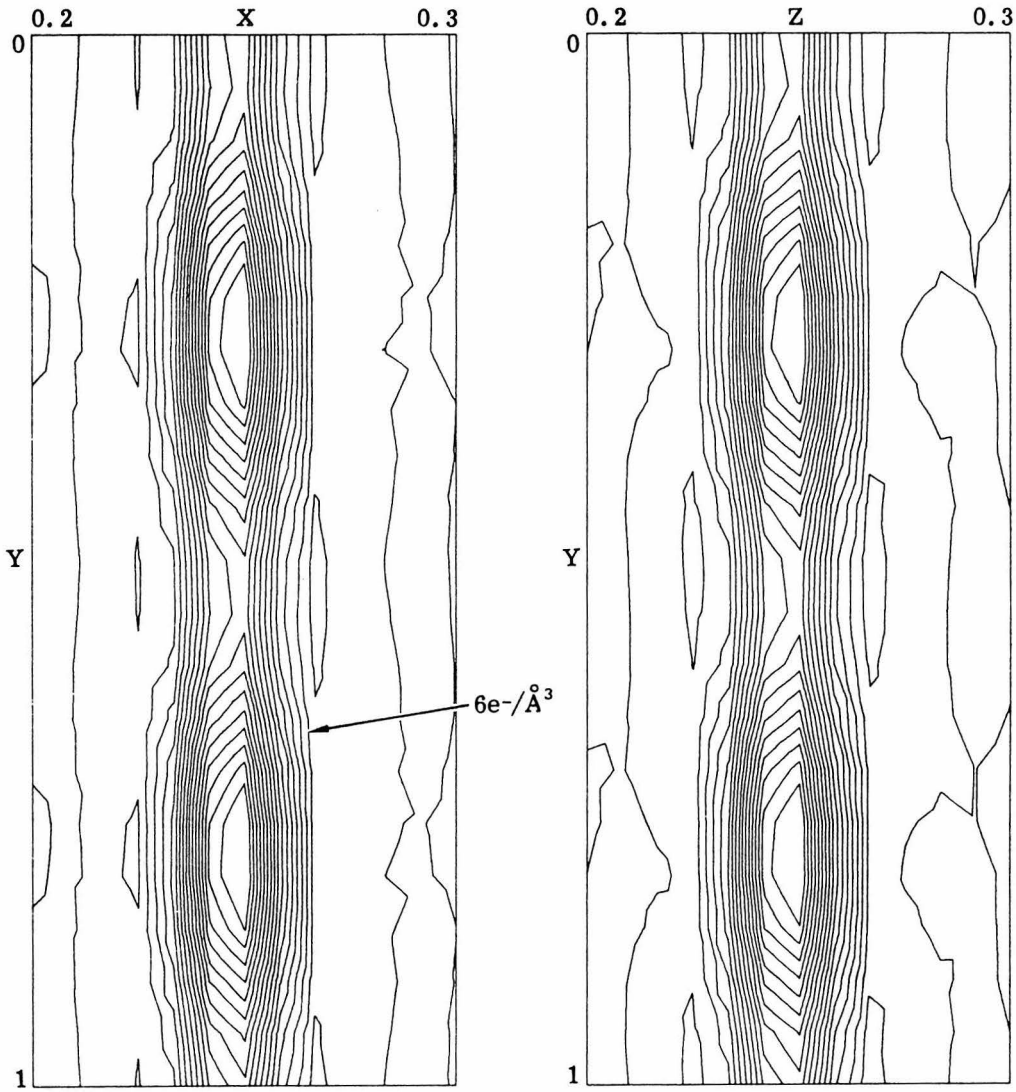
Difference Fourier Sections through Iodine Channel

Contoured at 0.5 electrons/$\mathring{A}^3$ intervals

------ negative contours

———— zero and positive contours

Figure 12

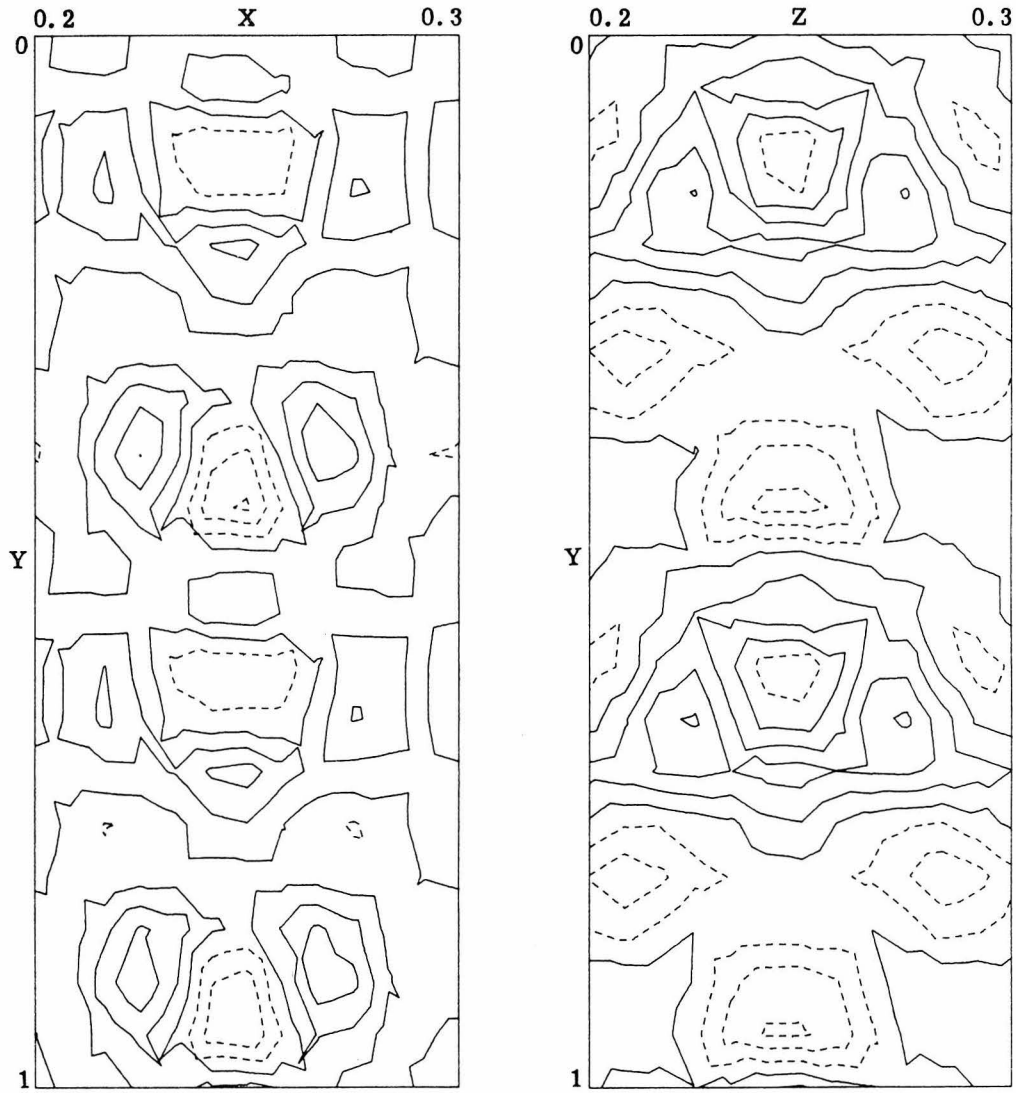


TTT_2I_3 (h.d.) at 19°K

Electron Density along Iodine Channel

Contoured at 6 electrons /Å³ intervals beginning at zero

Figure 13



TTT_2I_3 (h.d.) at 19°K

Difference Fourier Sections through Iodine Channel

Contoured at 0.5 electrons/$Å^3$ intervals

------ negative contours

——— zero and positive contours

Figure 14

Table XII

Maximum and Minimum Electron Density at 1/4, y, 1/4 in TTT_2I_3 (h.d.).

	~294° K	164° K	74° K	19° K	
Maximum	32.9	58.4	83.5	112.4	$e/Å^3$
Position*	0.28	0.29	0.28	0.34	
Minimum	12.9	26.9	35.3	55.0	$e/Å^3$
Position*	0.03	0.03	0.04	0.04	

*y, in fractional coordinates.

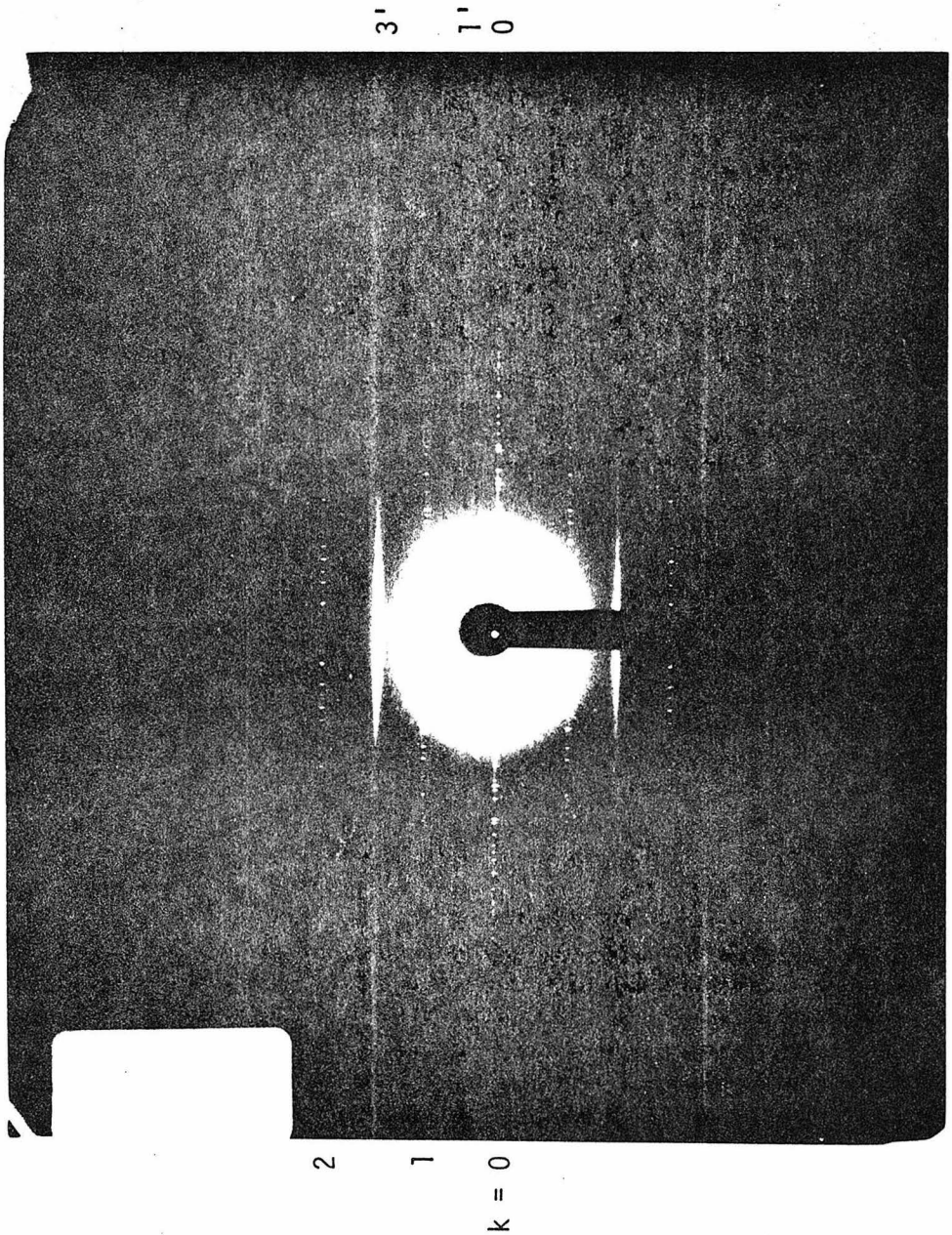
difference Fourier sections at 164° K, 74° K, and 19° K. The difference Fourier sections show that using two iodine atoms to represent the disordered iodide channel is not a perfect representation, especially at 19° K, but it is adequate. No additional information would be obtained by including more fractional iodine atoms to better represent the broad maximum. The root-mean-square (rms) displacements perpendicular to the channel at 19° K are ~0.1 Å. Small displacements off 1/4, y, 1/4 are possible, but the rms displacements are too small to suggest that any large kinks occur in the iodide chain.

The similarity of the iodide channels at 19° K, 74° K, and 164° K suggests that the "TTT" lattice sees only average, disordered iodide channels which never order. The TTT lattice does not appear to distort at low temperatures.

Temperature Dependence of the Diffuse Layer Lines

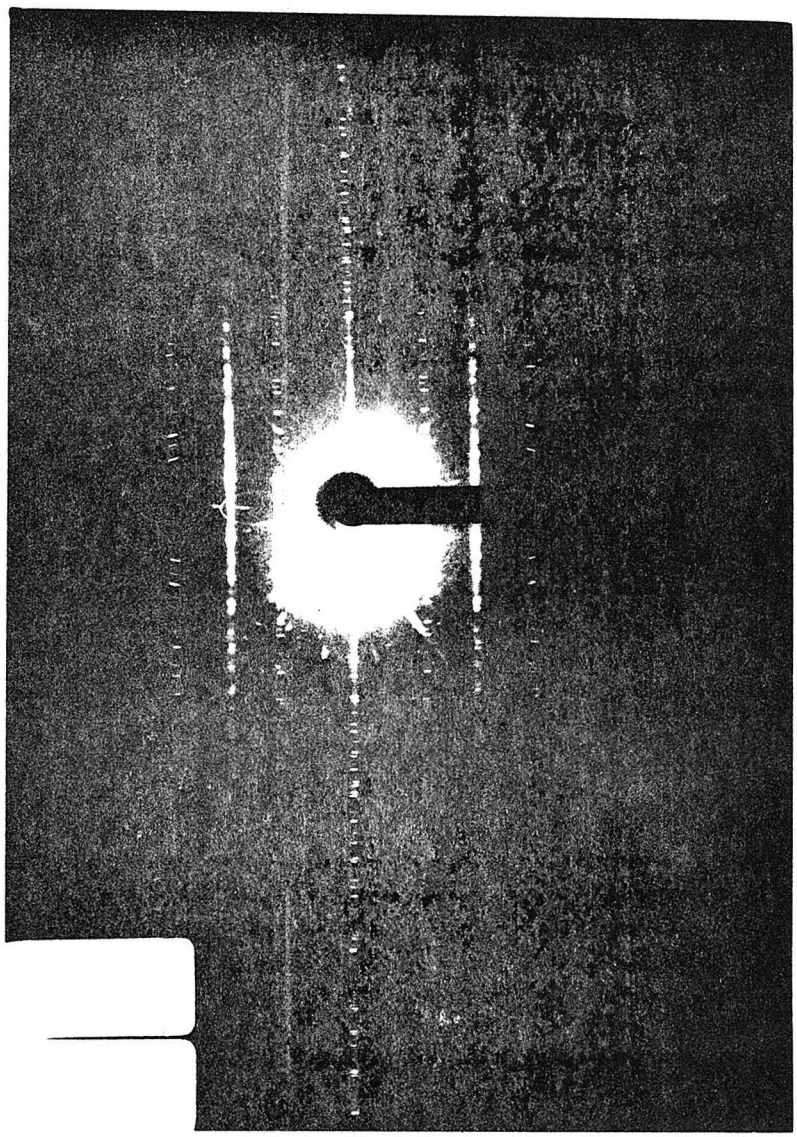
Although there is apparently no information in the TTT lattice (three-dimensional Bragg reflections) to suggest any phase transitions, the TTT lattice does not contain all of the structural information. The phase transitions could be related to changes that might only affect the diffuse layer lines. Figure 15 is a room-temperature X-ray oscillation photograph of a single crystal of TTT_2I_3 (h.d.) rotated about $\vec{b}$ and taken with nickel-filtered copper K_α radiation. The layer lines for the TTT lattice (b = 4.962 Å) are labelled on the left side of the photograph. Because the diffuse layer lines are incommensurate

with the TTT lattice, they do not really represent a supercell. However, for convenience the diffuse layer lines have been labelled as shown on the right side of the photograph. At room temperature there is very slight beading along the intense, diffuse, k = 3' layer line, but no beading on the other diffuse layer lines. The diffuse layer lines can be explained by the presence of one-dimensional chains of iodine atoms which are not correlated perpendicular to the chain direction. The beading on the k = 3' layer indicates that there is some very weak, short-range order between the chains. Lowering the temperature of the crystal could cause any of three effects to occur: (i) the chains could three-dimensionally order amongst themselves into a lattice incommensurate with the TTT lattice, (ii) the chains could order with respect to the TTT lattice causing the formation, probably, of a supercell, or (iii) the chains could remain disordered and uncorrelated. Figure 16 is an oscillation photograph about $\vec{b}$ of a TTT_2I_3 (h.d.) crystal at 120±10° K. The crystal had been rapidly cooled in a stream of cold N_2 gas. There is a definite increase of beading on the k = 3' layer, but no apparent beading on the other diffuse layers. A Weissenberg photograph of the k = 3' layer at ~120° K (Figure 17) shows that the increased beading is not due to additional ordering but to a loss of thermal motion. The size and shape of the diffraction 'spots' (blobs really) at 120° K are about the same as at room temperature indicating, still, only short-range chain-chain ordering. An X-ray photograph at ~120° K obviously will not give information about a phase transition at ~100° K.



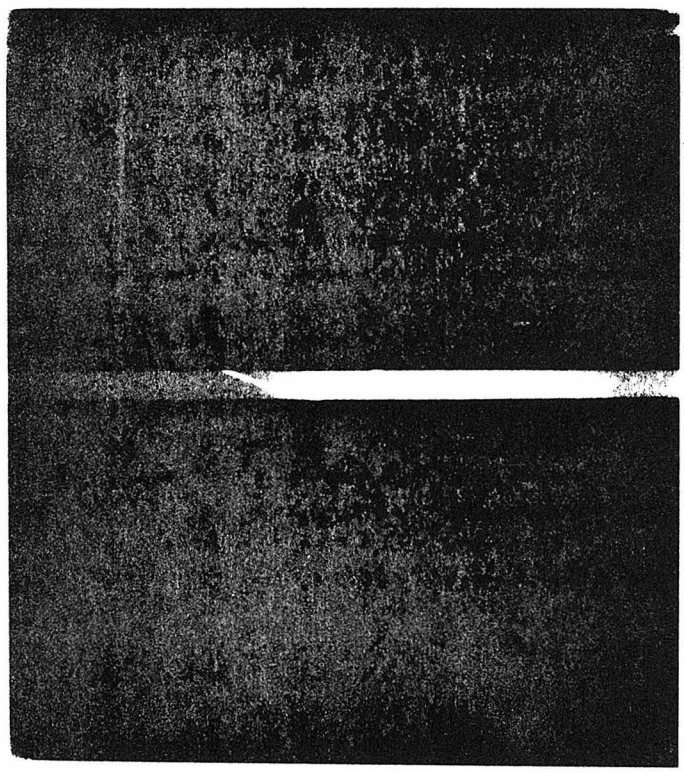
A Room Temperature X-Ray Oscillation Photograph of TTT_2I_3 (h.d.) (CuK_α)

Figure 15



An X-Ray Oscillation Photograph of TTT_2I_3 (h.d.) at ~120 ± 10° K (CuK_α)

Figure 16



A Weissenberg Photograph (k = 3')

of TTT_2I_3 (h.d.) at ~120 ± 10° K (CuK_α)

Figure 17

During the slow-cooling of the fifth TTT_2I_3 (h.d.) crystal (see the previous Experimental Section) the k = 3' layer was carefully monitored. In addition, a sixth crystal of TTT_2I_3 (h.d.) was put on the low-temperature diffractometer to monitor just the diffuse layer lines during slow-cooling. The sixth crystal was cooled in the following manner. From room temperature (~294° K) to 164° K the crystal was cooled between 2° per five minutes and 5° per forty-five minutes, with equilibration and peak scans every ten degrees. The phi-shaft was actually cooling at 0.1°/10 secs at the higher temperatures and 0.1°/25 secs at temperatures near 164° K. At 164° K omega scans, based on an orientation matrix for the 'spots' on the k = 3' layer, were collected for k = 1', 3', 5', 6', 7', and 9'. From 164° K to 76° K the temperature was turned down by 2° every five minutes, although the actual cooling rate at the phi-shaft was ~0.1°/35 secs. Every ten degrees the crystal was allowed to equilibrate and the peak scans were collected. At 76° K omega scans, based on an orientation matrix for 'spots' with k = 3', were again collected for reflections with k = 1', 3', 5', 6', 7' and 9'. From 76° K to 24° K, the lowest temperature attained with the sixth crystal, the temperature was turned down at a rate of 0.2° per five minutes. The phi-shaft was actually cooling at ~0.1°/45 secs. At 24° K omega scans of reflections with k = 1', 3', 5', 6', 7', and 9' were collected with an orientation matrix for 'spots' with k = 3'.

There is no evidence from the slow-cooling experiments with the fifth and sixth TTT_2I_3 (h.d.) crystals studied at low temperatures that

the beading on the diffuse layer lines ever collapses to sharp reflections corresponding to long-range, three-dimensional ordering. The iodide chains remained disordered with only short-range chain-chain order from 294° to 19° K. Patterson maps calculated from intensities of only diffuse layer 'spots' at 164°, 76°, and 27° K confirm that the diffuse layer lines are caused solely by scattering from the iodide chains.

Shown in Figures 18, 19, and 20 are scans at various temperatures of reflections on the diffuse layer lines.* Although the 33'4 certainly increases in intensity with decreasing temperature (Figure 18), the full-width at half-height (FWHH) remains about the same. At 136° K the FWHH is about 1.38° ω ($\pm$ ~.1° ω), at 96° K FWHH $\simeq$ 1.65° ω, at 48° K FWHH $\simeq$ 1.26° ω, and at 20° K FWHH $\simeq$ 1.38° ω. Figure 19 shows the effect of temperature on a different reflection, the 13'0. At room temperature with molybdenum K_α radiation the 13'0 cannot really be resolved with diffractometer scans, although it can be seen on a 135 hour, room temperature Weissenberg photograph taken with copper K_α radiation. With decreasing temperature the 13'0 gains in intensity, but the peak shape continues to indicate only short-range coherent scattering. The intensity gain with slow cooling is completely reversible. The room temperature scan of the 13'0 in Figure 19 was actually run after the crystal had been cooled to 24° K and warmed

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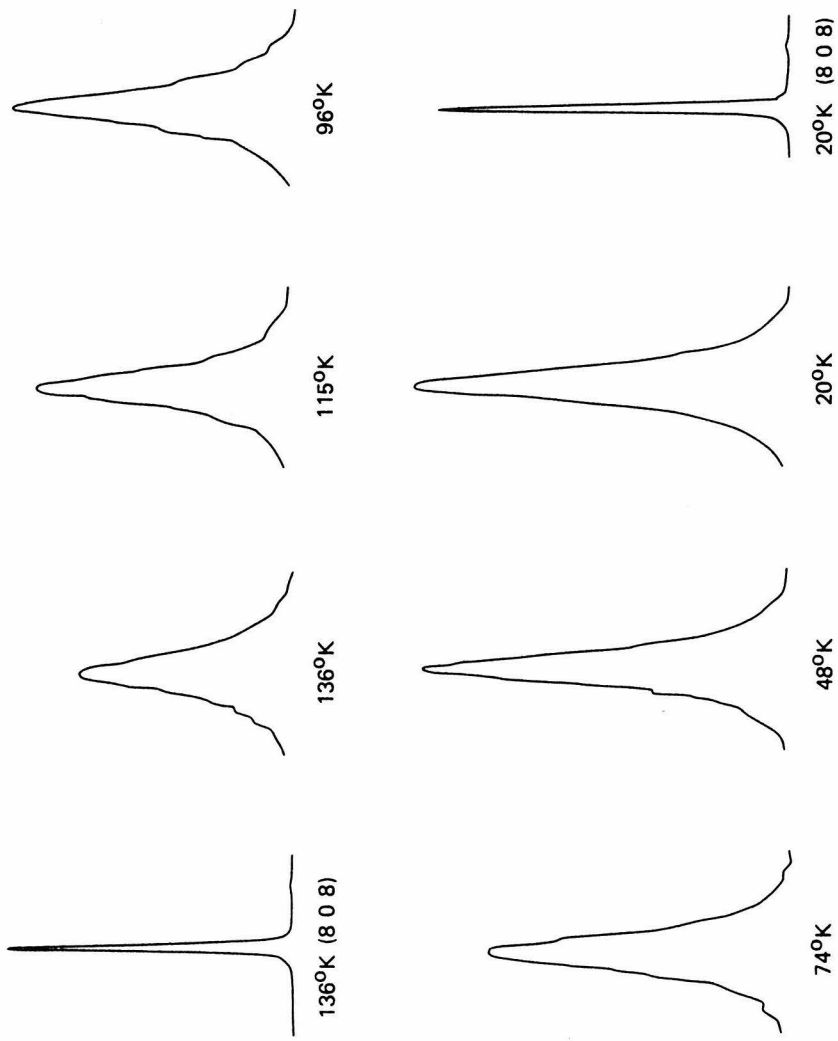
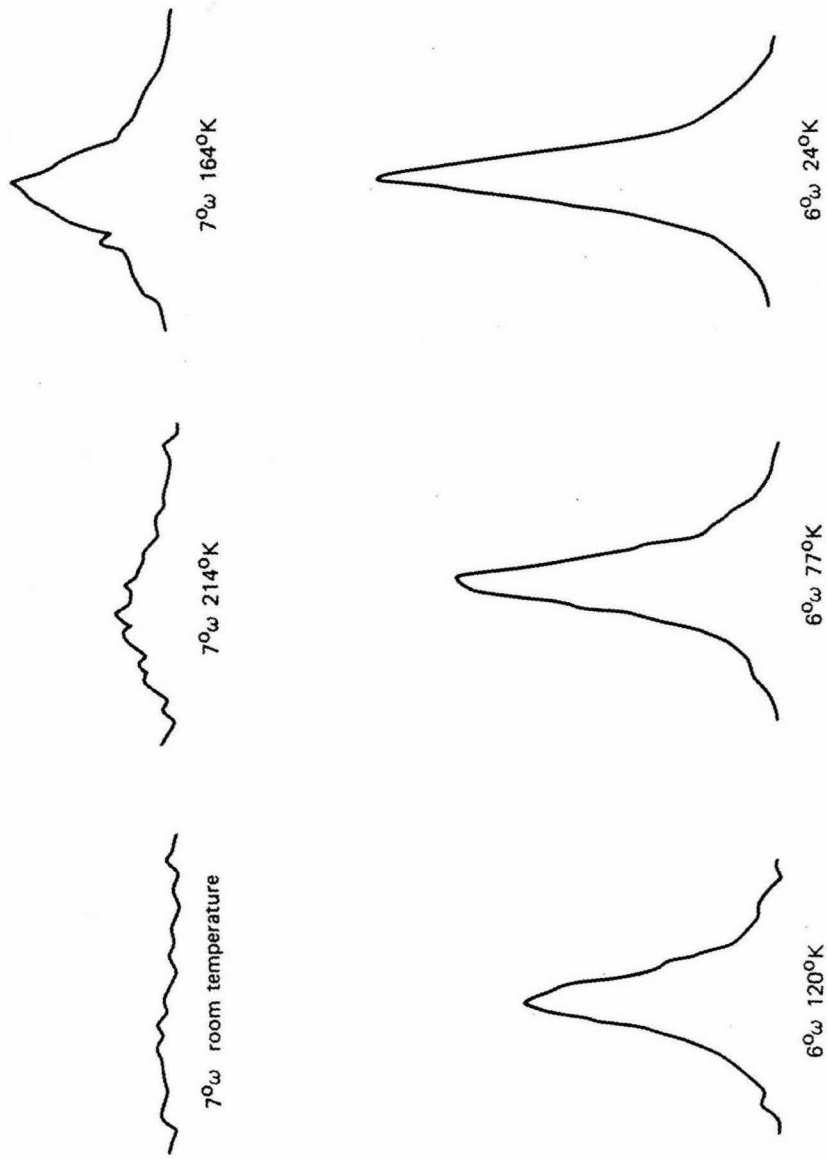
*The h and ℓ indices in Figures 18, 19, 20, 21, and 22 and references to them in the text refer to an A-centered TTT lattice. For comparison with C-centered TTT indices h and ℓ should be interchanged. In Figures 18 - 22 the index k is really k'.



A Selected "Diffuse" Reflection, 3 3 4, as a Function of Temperature at the ϕ-shaft (6.2^{o} omega scans)

The intensity scale for 3 3 4 is expanded by ten times that of the 8 0 8

Figure 18



TTT_2I_3 (h.d.) omega scans of 1 3 0 at various Φ-shaft temperatures

Figure 19

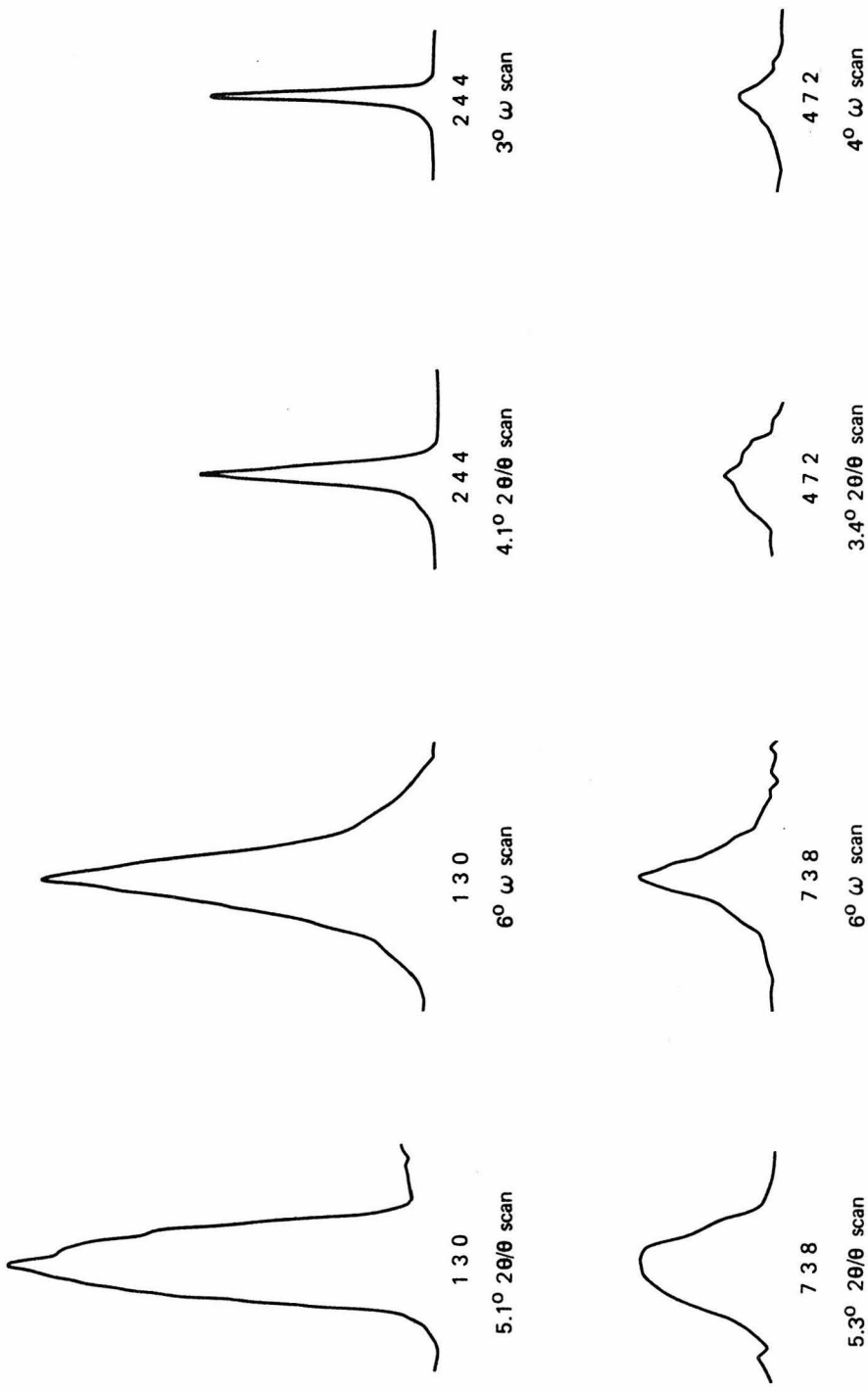

1 3 0
5.1° 2θ/θ scan
1 3 0
6° ω scan
2 4 4
4.1° 2θ/θ scan
2 4 4
3° ω scan
7 3 8
5.3° 2θ/θ scan
7 3 8
6° ω scan
4 7 2
3.4° 2θ/θ scan
4 7 2
4° ω scan
TTT2I3 (h.d.)
φ ~ 24°K

Figure 20

back to room temperature. Figure 20 shows scans of three reflections on the diffuse layer lines at 24° K and, for comparison, a TTT lattice reflection, the "2 4 4". The "2 4 4" is really 422 for the C-centered (Cmca) TTT lattice. The intensity scale for the diffuse reflections is expanded by five times that of the TTT lattice reflection. The full-widths at half-height for the omega scans are: 13'0, FWHH ~ 1.22° ω, 73'8, FWHH ~ 1.22° ω, 47'2, FWHH ~ 0.9° ω, "2 4 4", FWHH ~ 0.24° ± .05° ω, and for 808 (not shown in Figure 20), FWHH ~ 0.24° ± 0.05° ω. For 13'0, 73'8, and 47'2 the estimated error in measuring the FWHH is about ±0.10° ω. Figures 18-20 show that from 294° K to 19° K the iodide chains, even with very slow cooling, do not achieve long-range coherency.

Figure 21 is a plot of the integrated intensities from omega scans of several reflections on the diffuse layers and one hOℓ reflection as a function of temperature.* Figure 22 is a similar plot of the integrated intensities from omega scans of several TTT lattice reflections. Figures 21 and 22 are really a summary of the effect of slow-cooling on TTT_2I_3 (h.d.). Except for a possible anomaly at 85-90° K and a general leveling-off of intensities below about 40-50° K, with very slow cooling there is no evidence for a structural phase transition in TTT_2I_3 (h.d.) from ~294° K to 19° K. The TTT lattice remains orthorhombic with Cmca symmetry and does not form a supercell.

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*All of the scans in Figures 21 and 22 were run with a large, 5 mm collector aperture. A normal 1 mm collimator was used on the monochromator for the primary X-ray beam.

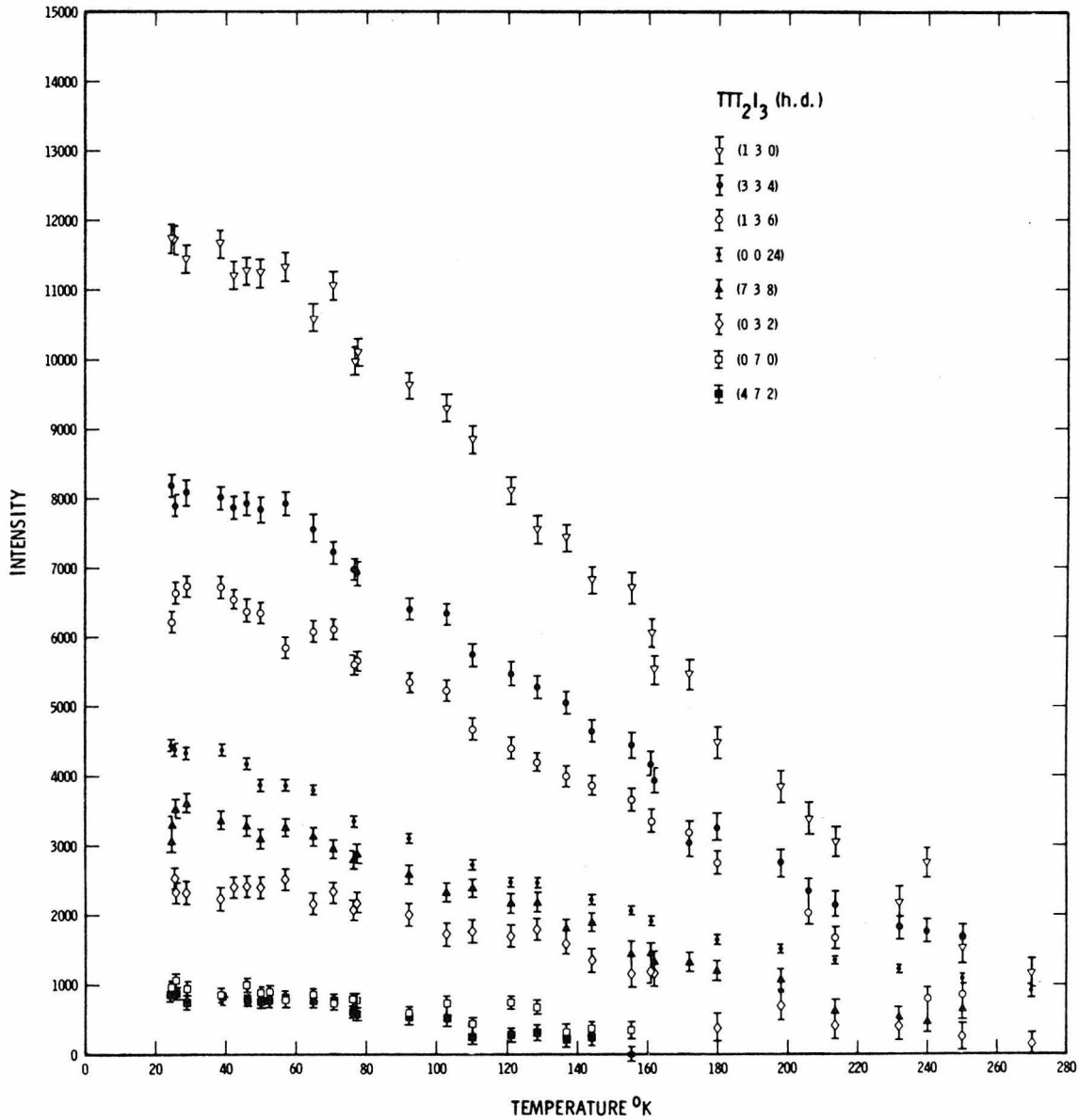

TTT2I3 (h.d.)
(1 3 0)
(3 3 4)
(1 3 6)
(0 0 24)
(7 3 8)
(0 3 2)
(0 7 0)
(4 7 2)
INTENSITY
TEMPERATURE °K
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280

Figure 21

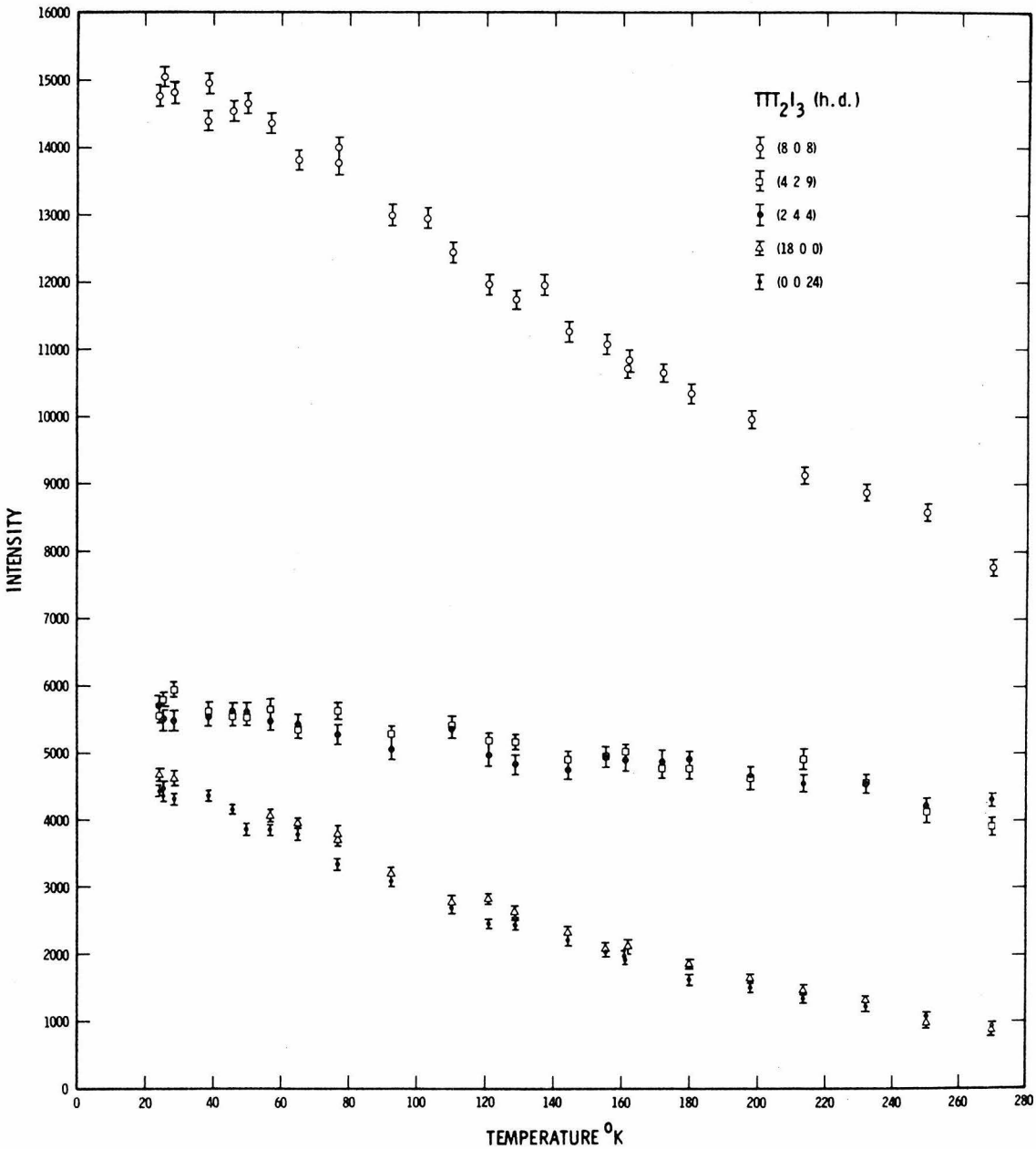

TTT2I3 (h.d.)
(8 0 8)
(4 2 9)
(2 4 4)
(18 0 0)
(0 0 24)
INTENSITY
TEMPERATURE °K
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
16000
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280

Figure 22

Reflections with k = 3' and k = 7' are incommensurate with the stacking axis of the TTT molecules (Table XIII). The diffuse layers with k = 1', 5', 6', and 9' apparently remain diffuse. No reflections from these layers were observed. The intensities of the reflections on the two diffuse layer lines, k = 3' and k = 7', do increase. But, reflections on these layers remain very broad and weak even at 19° K indicating no long-range three-dimensional ordering.

Table XIII

TTT_2I_3 (h.d.)

Reflections[b]	Number of Reflections	Unit Cell Parameters[a] a	b	c	Temperature[c]
hkℓ (Cmca)	22	18.259(6)	4.933(4)	18.341(8)	164° K
h3'ℓ hOℓ	5 7	18.266(9)	9.614(17)	18.342(13)	164° K
hkℓ (Cmca)	32	18.208(6)	4.924(2)	18.265(8)	76° K
h3'ℓ	8	18.212(28)	9.569(19)	18.252(43)	76° K
h3'ℓ hOℓ	8 9	18.215(7)	9.564(11)	18.268(8)	76° K
hkℓ (Cmca)	36	18.192(6)	4.923(3)	18.235(8)	24° K
h3'ℓ	10	18.158(31)	9.601(21)	18.230(52)	24° K
h3'ℓ hOℓ	10 14	18.193(6)	9.584(13)	18.238(8)	24° K
h7'ℓ hOℓ	4 14	18.195(6)	9.732(5)	18.238(8)	24° K

[a]Values in this table are from the sixth crystal used for low temperature studies and should not be compared to values from the fifth crystal (Table I). The sixth crystal was not as well centered. Cell edge lengths are from a symmetry-constrained (orthorhombic) least-squares fit of 2θ values.

[b]h and ℓ are the same as for the TTT lattice, Cmca.
k' is the diffuse layer index (Figure 15).

[c]phi-shaft temperature.

2.3 Discussion of the Diffuse Layer Lines

There are many causes for the appearance of diffuse scattering in the reciprocal space of seemingly ordered, three-dimensional crystals (22, 23). The causes can be broadly classified as from either thermal (dynamic) effects or structural (static) effects. The temperature-dependence studies of TTT_2I_3 (h.d.) suggest that the major cause of the diffuse layer lines is structural disorder. The anionic species in the channels of TTT_2I_3 are commonly assumed to be I_3^-, and that random shifts along $\vec{b}$ of the I_3^- units in the channels will cause the diffuse layer lines observed on the X-ray diffraction photographs (9, 24, 25). This is a fairly reasonable explanation. However, the room-temperature structure of low disorder TTT_2I_3 (JPL crystal) suggests that the disorder be best accounted for by assuming,in addition to chain slippage, the presence of small amounts of I^-, I_2, and possibly, other polyiodide species (26). Chemically this is quite reasonable. Iodine is known to form a variety of polyiodide species with strong inter-molecular interactions (27, 28, 29). A report by Beyeler in 1976 of the successful modeling of the X-ray diffraction pattern of the ionic conductor $K_{1.54}\ Mg_{0.77}\ Ti_{7.23}\ O_{16}$ (30) suggested that a similar approach might help to better understand the diffraction pattern for TTT_2I_3 (h.d.). In $K_{1.54}\ Mg_{0.77}\ Ti_{7.23}\ O_{16}$ the potassium cations are in channels. Beyeler modelled the potassium ions by assuming a random collection of cells of varying length and large displacements of the ions. He gave no details about how he calculated his final interference function.

The first model of the iodide chains in TTT_2I_3 (h.d.) assumes a collection of randomly occuring I_3^-, I_2, I^- spacings. Guinier (31) has shown how to calculate the interference function for such a model. For three spacings the distribution of these spacings is a sum of three delta functions $h(x) = p_1\delta(x-d_1) + p_2\delta(x-d_2) + p_3\delta(x-d_3)$. The probability of each spacing, d_j, occurring is p_j, and $p_3 = 1-p_1-p_2$. The crystal in real space is built from the convolution of h(x) with itself an infinite number of times and this function is z(x). The Fourier transform of z(x) gives the interference pattern of the crystal in one-dimensional reciprocal space. The transform of h(x) is

$$H(s) = \int h(x)\exp(2\pi isx)dx = \sum_j p_j\exp(2\pi isd_j) \quad . \qquad \text{Equation 1}$$

Therefore,

$$\text{transf } z(x) = Z(s) = 1 + H(s) + H^2(s) + H^3(s) + \ldots$$
$$+ H^*(s) + [H^*(s)]^2 + [H^*(s)]^3 + \ldots$$

If h(x) had been represented by a single delta function, ie. a lattice with a single repeat spacing a, then Z(s) would be the interference function (or diffraction pattern) for a one-dimensional grating and $Z(s) = 1 + 2\sum_{n=1}^{\infty}\cos(2\pi na)$. Since $\sum_j^N p_j = 1$, $|H(s)|$ (equation 1) is always less than one when $N > 1$ (except at $s = 0$) and so Z(s) is a geometric progression which can be expressed as

$$Z(s) = 2 \text{ Real } [\frac{1}{1-H(s)}] - 1 \ .$$

This is the same result that Wright obtained (32). Hendricks and Teller (33) and Méring (34) also calculated this same result but expressed Z(s) in the form

$$Z(s) = \frac{1-R^2}{1+R^2-2R\cos\phi} \qquad \text{Equation 2}$$

where $Re^{i\phi} = \sum_j p_j \exp(2\pi i s d_j) \equiv H(s)$ (35). On the basis of known bond lengths and van der Waal's radii (29,36), an I_3^- spacing would be ~10.1 Å, an I_2 spacing ~7 Å, and an I^- spacing ~4.3 Å for non-interacting species. Shown in Figure 23, as a function of $|\vec{s}|$ (35), are a series of computer-generated plots of Equation 2 in which the probabilities and spacings have been varied. The parameters for each plot are listed in Table XIV. These plots demonstrate that the positions and the intensities of the diffraction lines are sensitive to changes in the probabilities and spacings. Figure 24 is a 135 hour X-ray oscillation photograph of TTT_2I_3 (h.d.) rotated about $\vec{b}$. The photograph was taken in a cylindrical camera with monochromatized molybdenum K_α radiation. The film was wrapped in 0.005 inch aluminum and after development the back emulsion of the Kodak No-Screen X-ray film was removed. This oscillation photograph exhibits a weak k = 1' diffuse layer line, a weak k = 2' diffuse layer line next to but incommensurate with the TTT lattice line, a very strong k = 3' line with possibly two components, a weak k = 4' line again next to, but incommensurate with the TTT

Table XIV

Parameters for the Plots Shown in Figure 23

	I_3^-	I_2	I^-
	probability, spacing (Å)	probability, spacing (Å)	probability, spacing (Å)
A	0.80 , 10.1	0.10 , 7.0	0.10 , 4.3
B	0.50 , 10.1	0.30 , 7.0	0.20 , 4.3
C	0.70 , 9.8	0.25 , 6.5	0.05 , 4.3
D	0.70 , 10.0	0.25 , 6.7	0.05 , 4.2
E	0.70 , 10.1	0.25 , 7.0	0.05 , 4.3

The function plotted is $Z(s) = (1-R^2)/(1 + R^2 - 2R\cos\phi)$ for $R\exp(i\phi) = \sum_{j=1}^{3} p_j \exp(2\pi i s d_j)$.

p_j is the probability of spacing d_j occurring and $\sum_j p_j = 1$.

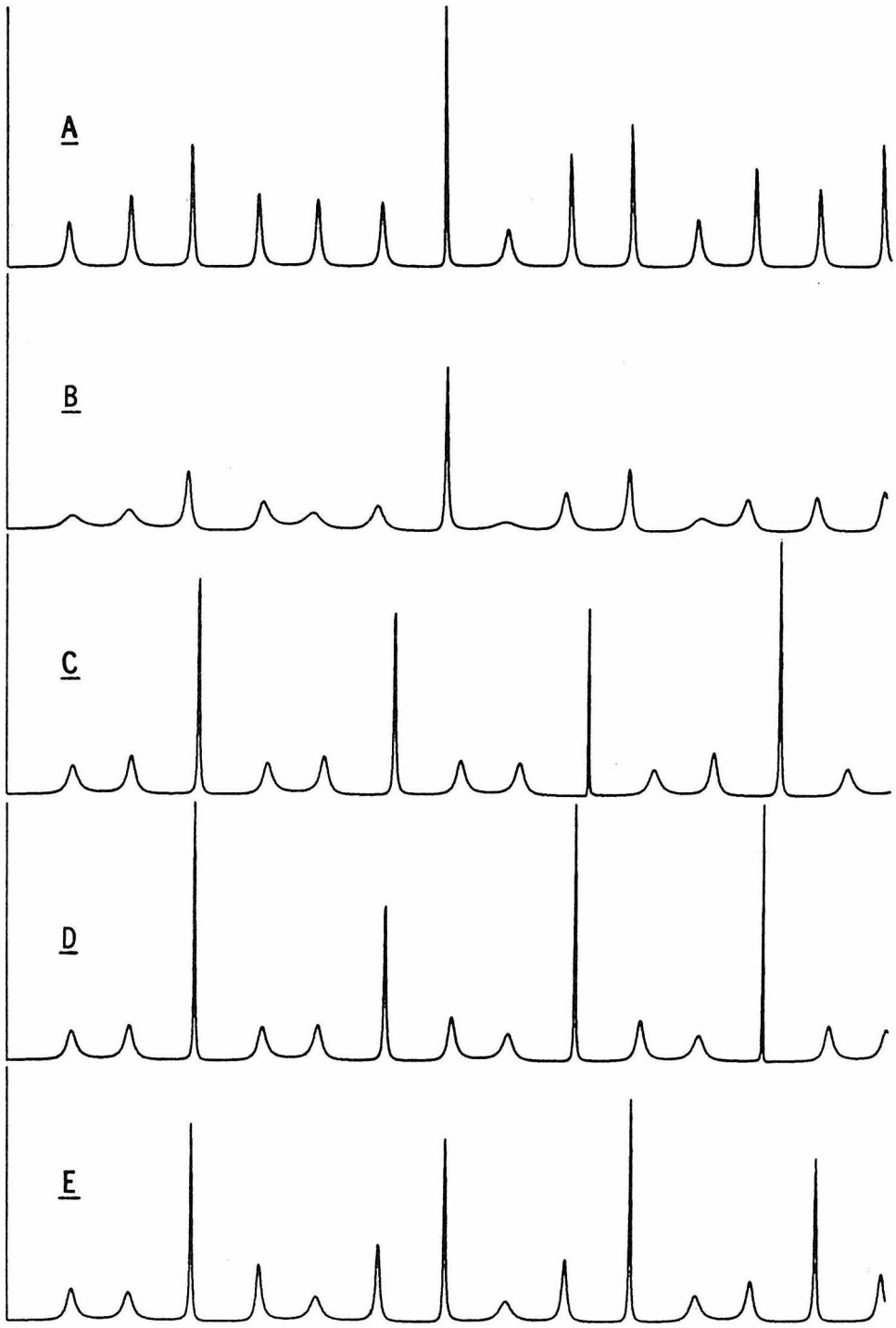
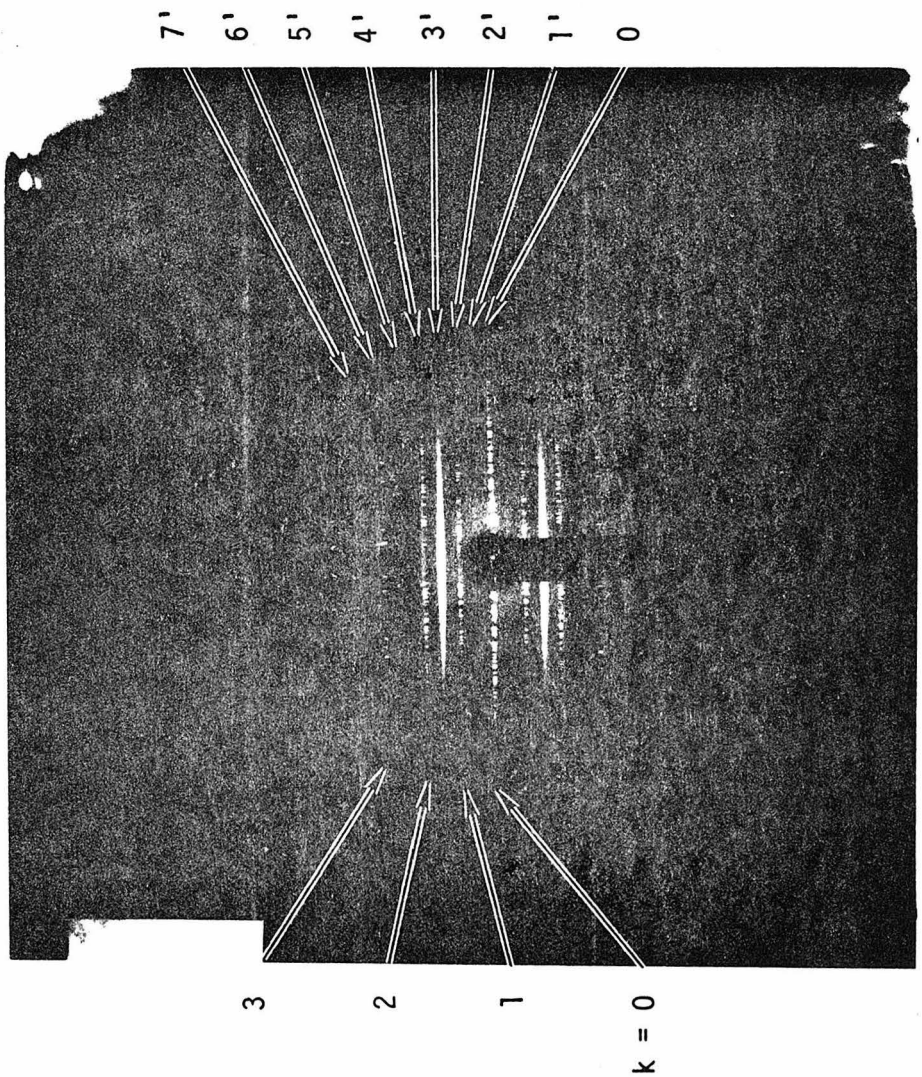


Figure 23

Interference function, Z(s) (Equation 2).



A Room Temperature X-Ray Oscillation Photograph of TTT_2I_3 (h.d.)

(135 hrs. monochromatized MoK_α)

Figure 24

lattice line, a k = 5' diffuse layer line, a moderately strong k = 6' line clearly displaced from the TTT line, a moderately strong k = 7' line, and two or three broad, very weak diffuse lines at higher angles. Although none of the plots in Figure 23 are an exact replication of the oscillation photograph, the similarities are encouraging.

Further improvements in the model ought to include the effect of slight atomic displacements (ie. "thermal" parameters or "temperature factors"), the effect of different spacings containing different amounts of scattering matter (ie. structure factors), and the effect, perhaps, of slight variations in the spacings and nearest-neighbor correlations. A model with different spacings for different iodide species is very similar to stratification in clays. Several people have worked out the expected diffraction patterns for clay with interstitial material. One of the more recent and fairly complete treatments of this problem has been published by Wright (32). His intensity expression is used here to model the diffraction pattern of the iodide chains in TTT_2I_3 (h.d.). This is a one-dimensional model and represents, essentially, the diffraction pattern expected for one infinitely long chain.

Wright has assumed in the derivation of his model that there is a basic layer with some spacing which represents the majority of the structure. But, the basic layers do not always come in perfect succession; occasionally there are layers of other material, with different spacings, in between the basic layers. Although this model allows for the

possibility of an I_3^- following an I_3^- in the chain, I_2 or I^- species would always be bordered on either side by I_3^-. For this model of an infinite chain the intensity would be given by the expression (32)

$$|A(s)|^2 = 2[\beta\beta^+/(1-\alpha)]_{real} - |F_b|^2 + p_1|F_1|^2 + p_2|F_2|^2 \qquad \text{Equation 3}$$

where

$$\beta = F_b + p_1F_1e^{i\phi 1/2} + p_2F_2e^{i\phi 2/2}$$

$$\beta^+ = F_b^* + p_1F_1^*e^{i\phi_1/2} + p_2F_2^*e^{i\phi_2/2}$$

and $\alpha = \sum_k p_k e^{i\phi_k}$.

p_k are probabilities and $\sum_k p_k = 1$. F_b is the structure factor for the basic layer, in this case I_3^-. F_1 and F_2 are structure factors for I_2 and I^-. When an I_3^- follows an I_3^- the structure factor for the nonexistent interstitial material is zero, but there is a term in α for the probability of an I_3^- following an I_3^-. ϕ_k is the phase shift due to the spacing of an I_3^- plus the spacing for the k species. Included in the structure factors are terms of the form $\exp(-B\sin^2\theta/\lambda^2)$ to account for thermal motion of the atoms (37). Preliminary calculations of Equation 3 showed that I_3^- following I_3^- is a prominent feature of the iodine chains. Shown in Figure 25a are computer-generated plots of Equation 3.

The parameters for each plot are listed in Table XVa. The effect of a slightly asymmetric I_3^- is negligible. The probabilities of each species primarily determine the intensities of the various lines, although the spacings do affect the intensities. The plots show basically the same diffraction pattern as in Figure 24. The plots indicate that 70-80% of the I_3^- will have I_3^- as nearest neighbors, but there is a small percentage of I_2 and I^- present.

The oscillation photographs have broad diffraction lines, especially at high angles, which the plots in Figure 25a do not have. Two effects could cause the observed broadening. The mosaic blocks in the crystal could be very small or the spacings of the iodide species could be variable. Because the TTT lattice in TTT_2I_3 (h.d.) gives rise to very normal, sharp reflections, there is no reason to assume unusually small mosaic blocks. However, the spacings of the iodide species could, realistically, be quite variable. I_3^-, I_2, and I^- are known to form "polyiodide" species with a wide range of inter- and intramolecular I-I distances (27,28,29,38,39). For the case when the variations in the spacings are much smaller than the average spacings and the variations have a normal distribution about the average spacings, Wright has derived the following modifications to Equation 3. For spacings d_k (d_k is the basic plus interlayer spacing) with a deviation of Δ_k ($\Delta_k << d_k$), then

$$\alpha = \sum_k p_k \exp(2\pi i s d_k) \exp(-2\pi^2 s^2 {\Delta_k}^2)$$

Table XVa

Parameters for the Plots of the Wright Model

Figure 25a - No deviations in the spacings

Constants in all five plots $D_{II}(I_2) = 2.70$ Å

spacings: $I_3^- + I_2 = 16.7$ Å $I_3^- + I^- = 14.3$ Å $I_3^- + 0 = 9.9$ Å *

A

asymmetric I_3^- (I_a I_c I_b) I_a-I_c = 2.83 Å I_b-I_c = 3.04 Å

$B(I_a) = 8.0$ $B(I_b) = 10.0$ $B(I_c) = 2.0$ $B(I_2) = 4.0$ $B(I^-) = 3.0$

probabilities: $I_3^- + I_2$, 0.15 $I_3^- + I^- = 0.05$ $I_3^- + 0$, 0.80

B

symmetric I_3^- I_a-I_c = I_b-I_c = 2.92 Å

$B(I_a) = B(I_b) = 8.0$ $B(I_2) = 4.0$ $B(I^-) = 3.0$

probabilities: same as in A

C

asymmetric I_3^- (same bond lengths as in A)

$B(I_a) = 3.0$ $B(I_b) = 4.0$ $B(I_c) = 2.0$ $B(I_2) = 4.0$ $B(I^-) = 6.0$

probabilities: $I_3^- + I_2$, 0.15 $I_3^- + I^-$, 0.15 $I_3^- + 0$, 0.70

D

symmetric I_3^- (same bond lengths as in B)

$B(I_a) = B(I_b) = 3.0$ $B(I_c) = 2.0$ $B(I_2) = 4.0$ $B(I^-) = 6.0$

probabilities: same as in C

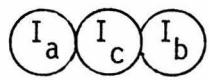
---

* I_3^- are nearest neighbors

Table XVb

Parameters for the Plots of the Wright Model (32)

Figure 25b - With deviations in the spacings

Constants in all four plots; asymmetric I_3^- 

I_a-I_c = 2.87 Å
I_b-I_c = 2.97 Å

$B(I_a) = B(I_b) = 2.0$ $B(I_c) = 1.0$ $B(I_2) = 3.0$ $B(I^-) = 3.0$ $D_{II}(I_2) = 2.70$Å

E			
Spacings:	$I_3^-+I_2$ = 16.7 Å	$I_3^-+I^-$ = 14.0	I_3^-+0 = 9.6*
Deviations:	0.5 Å	0.3	0.3
Probabilities:	0.18	0.04	0.78
F			
Spacings:	$I_3^-+I_2$ = 16.7 Å	$I_3^-+I^-$ = 14.3	I_3^-+0 = 10.0*
Deviations:	0.5 Å	0.3	0.3
Probabilities:	0.18	0.04	0.78
G			
Spacings:	$I_3^-+I_2$ = 17.0 Å	$I_3^-+I^-$ = 14.3	I_3^-+0 = 9.6*
Deviations:	0.5 Å	0.3	0.3
Probabilities:	0.18	0.04	0.78
H			
Spacings:	$I_3^-+I_2$ = 16.7 Å	$I_3^-+I^-$	I_3^-+0 = 9.7*
Deviations:	0.5 Å		0.3
Probabilities:	0.20	0.0	0.80

* I_3^- are nearest neighbors.

Figure 25a

Plot of the Wright Model (see Table XVa)

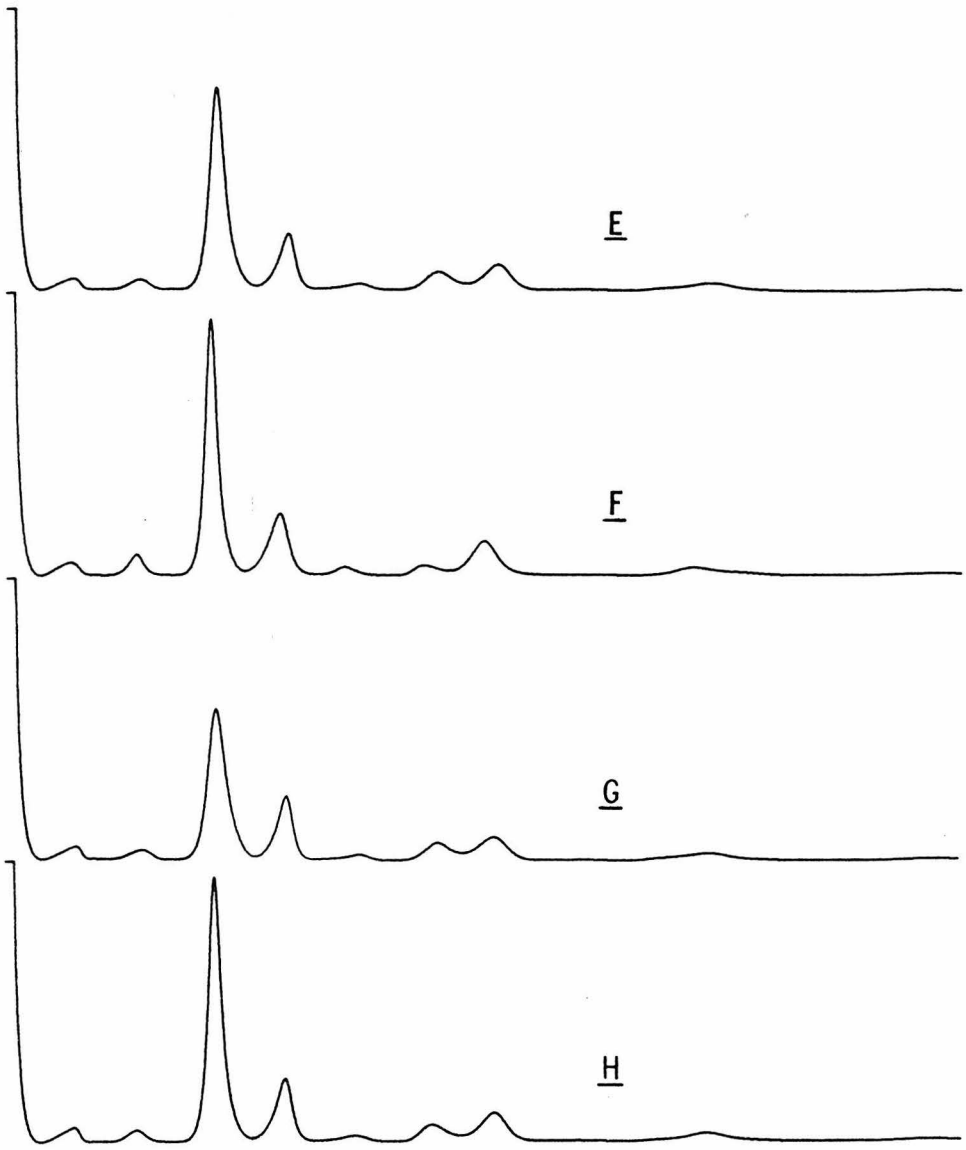


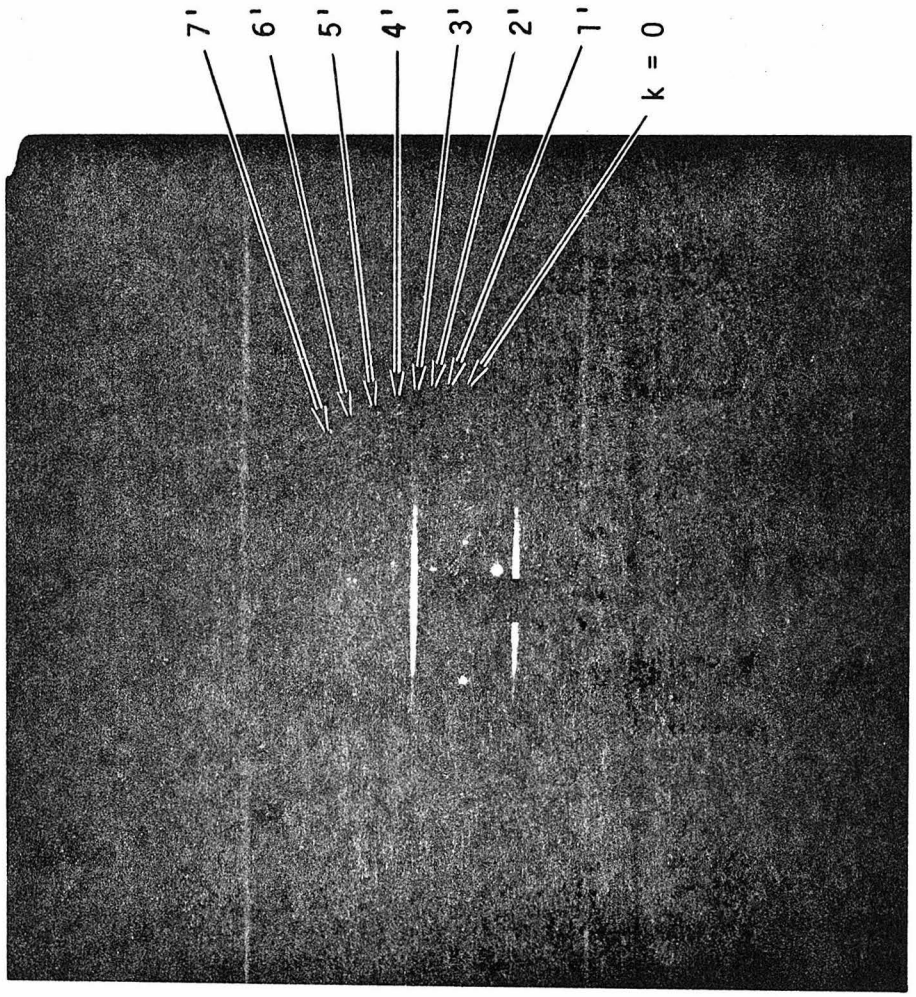
Figure 25b

Plot of Wright Model (see Table XVb)

$$\beta \approx F_b + \sum_k p_k F_k \exp(i\pi s d_k)\exp(-\pi^2 s^2 \Delta_k{}^2/2)$$

and $\phi_k \equiv 2\pi s d_k$ ($|\vec{s}| \equiv s = (\frac{2\sin\theta}{\lambda})$).

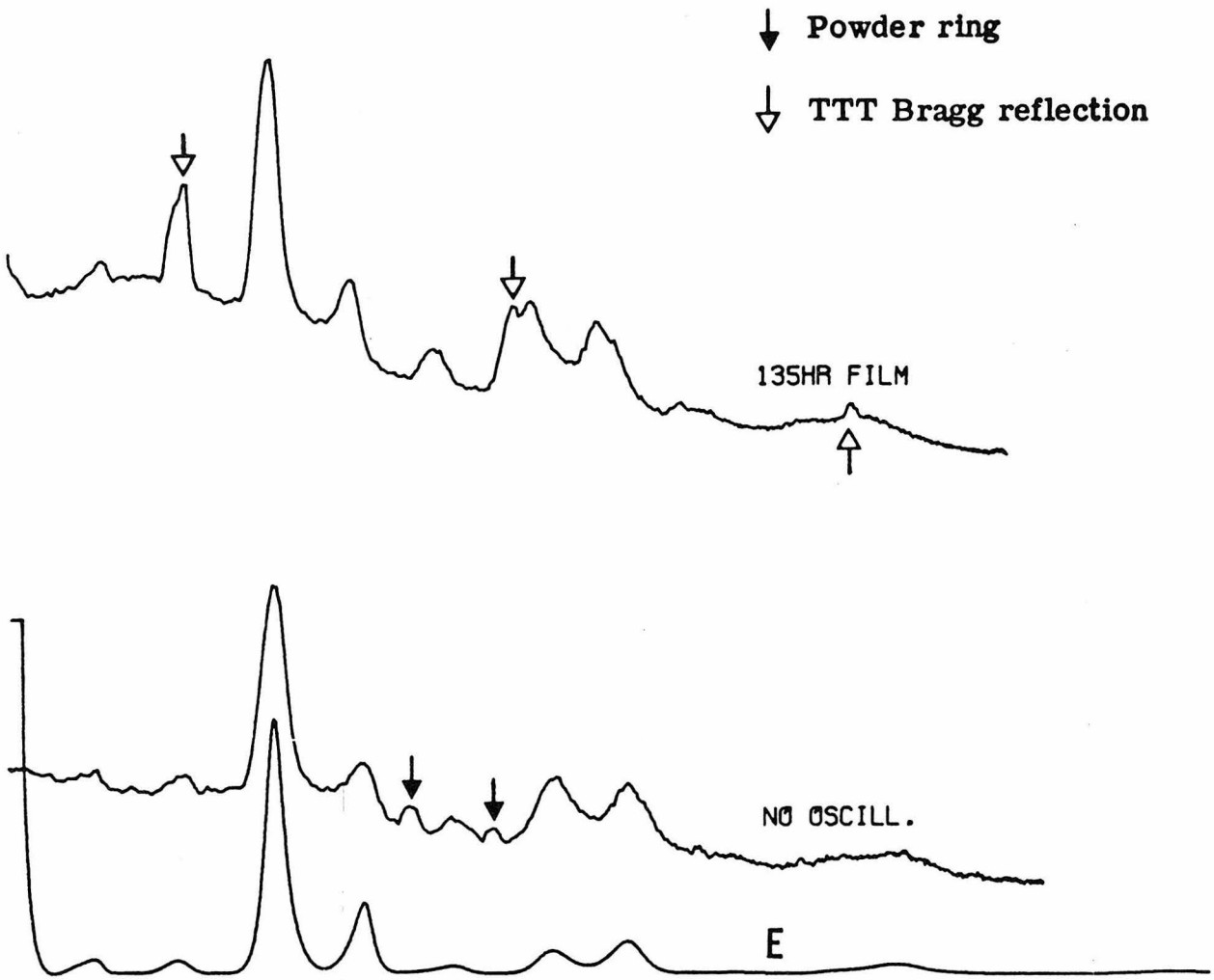
This treatment assumes that the deviations, Δ_k, will not cause a change in the structure factors. For the iodide chain this is reasonable, because the Δ_k are being used to represent the deviations in intermolecular spacings caused by variable amounts of interaction between iodide species. Shown in Figure 25b are computer-generated plots of Equation 3 but small deviations for the spacings have been included. Table XVb lists the parameters for the plots shown in Figure 25b. Not only do small deviations in the spacings cause broadening of the peaks at high angles, but the deviations seem to act as a "smoothing" function. With small spacing deviations Equation 3 is fairly insensitive to small changes in the other parameters. (Compare the changes in the parameters listed in Table XVb with the plots of Figure 25b,) Figure 26 is an X-ray photograph of TTT_2I_3 (h.d.) taken as the photograph in Figure 24 was with monochromatized molybdenum K_α radiation. The Kodak No-Screen X-ray film was wrapped in 0.005 inch aluminum and after developing the back emulsion was removed. This is a 72.6 hour exposure of a stationary crystal with a cylindrical camera. (The powder rings are not from the TTT_2I_3 (h.d.) crystal.) Optical film scans were made of the photographs in Figures 24 and 26 and of three other oscillation photographs taken under the same conditions but with different exposures (40). Figure 27 shows two of the film scans plotted as a function of $|\vec{s}|$. The



A Stationary X-Ray Diffraction Photograph of TTT_2I_3 (h.d.)

(monochromatized MoK_α, 72.6 hrs, ~294° K)

Figure 26



Comparison of Optical Film Scans with the Wright Model (Curve E, Figure 25b).

Figure 27

optical density plotted for the 135 hour exposure is an average of ten 0.1 mm scans of a 1 mm strip parallel to b. The optical density plotted for the 72.6 hour exposure, stationary photograph is an average of five 0.1 mm scans of a 0.5 mm strip parallel to $\vec{b}$. Also in Figure 27 is plot E of Figure 25 b. Plot E (the parameters are listed in Table XVb) shows all of the major features seen with the optical film scans. Although the fit may not be perfect, this one-dimensional model of the structure of the iodide chains can explain all of the major features of the TTT_2I_3 (h.d.) diffuse diffraction pattern. Although not seen with the film scans, the diffuse layers k = 3' and k = 7' actually consist of two components. This can be explained by the presence of two average spacings for I_3^- in the chains, for example I_3^- spacings of 10.0 Å and 9.6 Å.

Although the model is not perfect, in general it shows excellent agreement with the observed diffraction pattern. The agreement is good enough to say that, besides I_3^-, there is some finite amount of I_2 and probably a small amount of I^- present in the channels. This is a different conclusion from that of Isett and Perez-Albuerne (41). They interpret their Raman data as indicating the presence of less than 2% I_2 in Kodak crystals. The structural report by Smith and Luss and their descriptions of their X-ray photographs suggest, however, that the Kodak crystals are similar to the JPL crystals structurally. The presence of small amounts of I_2 and I^- in the channels would certainly explain why the iodide chains never three-dimensionally order. Although

at higher temperatures there is undoubtedly dynamic disorder, there is also, built into the structure, static disorder. The occasional mistake of an I_2 or I^- in the channel would prevent any long-range chain-chain ordering even at low temperatures.

From the information reported by Kaminskii, et al., (42) for Chernogolovka crystals and the diffuse X-ray scattering experiments done by Megtert, Pouget, Comès and Fourme on Chernogolovka crystals at low temperatures (43) the model presented here may not be a valid description of the Chernogolovka crystals. Some caution should be used in assuming that this model is completely valid for any TTT_2I_3 other than for TTT_2I_3 (h.d.) crystals grown at JPL since it is apparent that crystallization conditions can strongly effect the iodide composition of the resulting crystals.

2.4 Conclusions

The results of this study on TTT_2I_3 (h.d.) crystals grown at JPL are as follows:

(i) The room-temperature structure of the TTT lattice in TTT_2I_3 (h.d.) is the same as reported by Smith and Luss (9).

(ii) There is primarily I_3^- present in the channels, but I_2 and I^- are also occasionally present causing "mistakes" in the chains and preventing long-range chain-chain coupling.

(iii) With very slow cooling the TTT lattice in TTT_2I_3 (h.d.) apparently shows no structural phase transition to 19° K.

(iv) With very slow cooling the iodide chains never order which is consistent with (ii).

However, as mentioned in the Experimental Section for the low-temperature structures, all of the temperature-dependent data was collected on two crystals of TTT_2I_3 (h.d.), the fifth and sixth crystals studied. It might be of interest to mention what happened to the first four crystals.

The first crystal was cooled at a rate which would have cooled the crystal from 294° to 20° K in about 15-24 hours. The crystal shattered at 80-90°. The only piece of the crystal which could be found after warming to 294° K was the end of the crystal which was still firmly attached to the glass fiber.

The second crystal was cooled about twice as slowly, but cracked at ~90° K during the cooling. X-ray photographs of the crystal after warming to room temperature confirmed that the crystal really had split and remained split at room temperature.

The third crystal was coated with G. E. varnish after it was mounted on the glass fiber. It was cooled at a much slower rate. From 294° to ~90° K the temperature was lowered at ~1° per 5-10 minutes. From ~90° to 27° K the temperature was lowered at ~0.1° per 5 minutes. The crystal survived to the lowest temperature attained, ~27° K. During the data collection at 27° K the check reflections exhibited substantial decay.

Because a complete, reliable data set was not obtained from the third crystal, a fourth crystal, also coated with G. E. varnish, was cooled. This crystal was cooled rapidly from ~294° K to 27° K in about four hours. After 70 hours of data collection the check reflection intensities became very erratic, suggesting the structure was unstable and was changing with time.

The most reliable data collected from the third and fourth crystals were merged to form an almost complete data set. Solution of the structure using this data set suggested that the end ring of the TTT molecule was substantially bent away from planarity with the rest of the molecule. At room temperature the tilt of the end ring away from planarity is ~1° (±.2°). This same tilt was observed at 164° K, 74° K, and 19° K with the good data from the fifth crystal. However, with the combined data set from the third and fourth crystals, the

end ring appeared to be tilted ~3° (±0.2°) away from the planarity of the rest of the TTT molecule. It is not known whether this is the result of the fast cooling or of a systematic error in the data caused by merging data sets from crystals cooled at different rates. The k = 3' reflections observed with the fourth crystal also showed differences from the fifth and the sixth crystals. For the fifth and sixth crystals, reflections with h odd, k = 3' (h and ℓ here refer to the C-centered TTT lattice) were always absent. There were very, very weak intensities for reflections with h odd, k = 3' collected from the fourth crystal.

Although the data from the third and fourth crystals are somewhat unreliable and the third and fourth crystals were the only ones coated with G. E. varnish, the possibility still exists that cooling rate may affect the structure. Point-by-point sampling of reciprocal space with a diffractometer is extremely inefficient and time-consuming. It is possible that there was additional information such as satellites in regions of reciprocal space which were not scanned. The loss of the first two crystals may suggest the existence of a structural phase transition. Crystals of TTT_2I_3 (h.d.) are often reported to break on cooling (8). Measurement of the transport properties on crystals cooled at very slow rates have not been done.

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Goodness-of-fit = $[\sum w(|F_o|^2 - |F_c|^2)^2/(N-P)]^{1/2}$

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Chapter 3

Structure of (Tetrathiotetracene)-(Iodide)

Slight variations in the crystallization conditions of the tetrathiotetracene (TTT)-iodine system can lead to variations in the amount of disorder in TTT_2I_3 and, also, to other phases (1,2,3). When semiconducting crystals with a physical morphology very similar to metallic TTT_2I_3 were obtained at JPL, it was of interest to determine why the material was semiconducting (Appendix B) rather than metallic. To help elucidate why the material was semiconducting, a crystal structure determination was undertaken.

Experimental

The crystals of this phase were usually very thin, fragile needles with golden reflections. The density was measured by flotation to be 2.09 g/cm^3. Initial X-ray oscillation photographs, taken with the crystals rotated about their needle axes, showed an ordered structure with a plethora of layer lines which could not be indexed on the basis of a single lattice. At least ten crystals were examined by X-ray photographs and all exhibited an identical diffraction pattern. The diffraction pattern can be indexed by assuming two interacting lattices. (This is discussed in more detail later.) It was decided that the lattice with the repeat spacing of about 3.64 Å along the needle axis would be studied first.

Initial X-ray photographs of this lattice suggested a monoclinic cell. However, careful centering of fifteen reflections with a beam-splitter on a General Electric quarter-circle diffractometer and comparison of the integrated intensities of "equivalent" reflections confirmed that the unit cell chosen from the photographs actually has C-centered triclinic symmetry. All possible hk0 reflections to 2θ = 155.0° were collected with 1° per minute 2θ-θ scans on an automatic General Electric quarter-circle diffractometer using nickel-filtered copper K_α radiation. Backgrounds were collected for thirty seconds on each side of a scan. Equivalent Friedel-related reflections were combined by taking a weighted average of the F_o^2 (4). Weights were based on counting statistics and no more than two observations contributed to a weight. The structure in projection was solved from the two-dimensional, UVO Patterson projection. Partial refinement of the projection indicated the stoichiometry as TTTI (1:1) in agreement with the measured density. The crystal had dimensions of 0.83 mm x .008 mm x .517 mm (Table I). Absorption corrections (5) (μ = 212.875 cm^{-1}) were applied to the data set and full-matrix least-squares refinement continued until the refinement converged.

A complete three-dimensional data set for c = 3.643 Å was collected, as before, with 1° per minute 2θ-θ scans using nickel-filtered copper radiation on a General Electric quarter-circle diffractometer. Thirty second backgrounds were collected on both sides of a scan. Equivalent Friedel-related reflections were combined to yield a data set of 1620 reflections of which 1512 had $F_o^2 > 0$.

Table I

Crystal Data TTTI (Lattice 1, c = 3.643 Å)

a = 13.028(2) Å	α = 90.81(1)°	(λ = 1.5418 Å)
b = 16.445(2)	β = 96.11(1)	
c = 3.643(1)	γ = 91.11(1)	

V = 776 $Å^3$ Z = 2 F.W. = 479.4

d_c = 2.053

d_m = 2.09(3)

Triclinic, Space group $C\bar{1}$

Linear absorption coefficient (CuK_α), μ = 212.875 cm^{-1}.

Crystal dimensions 0.083 mm x 0.008 mm x 0.517 mm.

The same crystal used to collect the hk0 data was used for the complete three-dimensional data collection. Absorption corrections for the stoichiometry TTTI (μ = 212.875 cm^{-1}) were applied to the complete data set. The z coordinates of most of the atoms were obtained from the three-dimensional Patterson map. Iodine and sulfur atomic scattering factors were corrected for anomalous dispersion, and the real parts ($f_0 + \Delta f'$) were used in the structure factor calculations (6). After the positions of all the atoms (except hydrogens) were determined, the structure was refined by the full-matrix least-squares method. The weights used in the least-squares refinement were based on counting statistics. On a low-angle difference Fourier map of the approximately refined structure, very large, weak blobs of electron density were seen in positions that were geometrically correct for hydrogen atoms. The hydrogen atoms were included in the final least-square cycles, but were not refined. During the final least-square cycle all shifts were less than one-third of the corresponding standard deviation. Final atom coordinates and temperature factors are listed in Table II. The full matrix least-squares refinement converged to R = 0.102, with the goodness-of-fit = 4.7 for the complete data set (7). For 1132 reflections with $F_o^2 \geq 3\sigma(F_o^2)$, R = 0.081.

Discussion

Shown in Figure 1 and listed in Table III are bond lengths and bond angles, and their estimated standard deviations (assuming isotropic

Table IIa

Refined Atomic Coordinates for TTTI (Lattice 1, c = 3.643 Å)

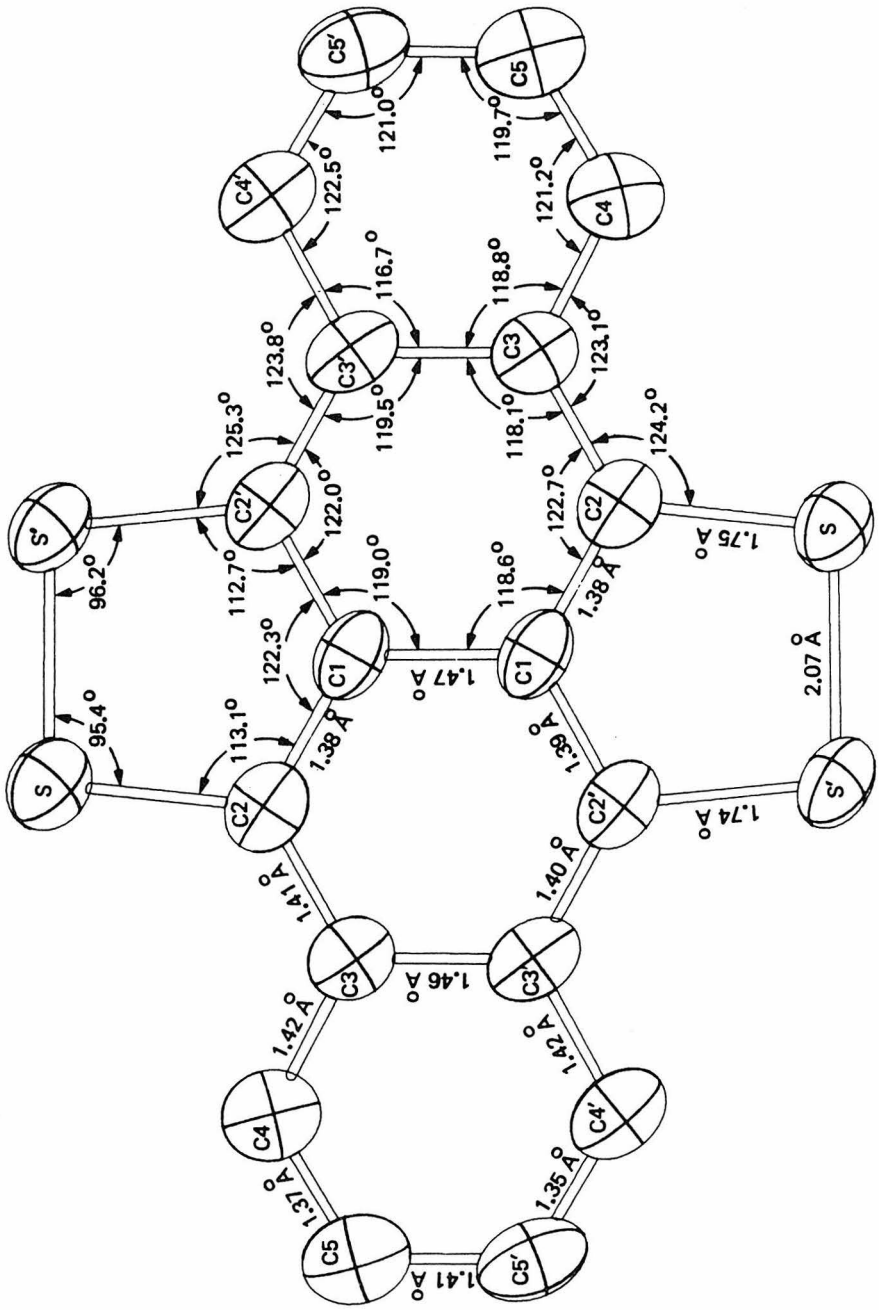
	X	Y	Z
I	0	0	0
S	.25896(17)	.06298(14)	.94596(81)
S'	.25951(17)	-.05920(14)	1.08012(81)
C1	.44396(60)	.00078(53)	1.01076(291)
C2	.39217(63)	.07140(52)	.91656(261)
C2'	.39269(63)	-.07028(53)	1.09972(252)
C3	.44302(67)	.14283(51)	.81213(253)
C3'	.55460(65)	.14147(51)	.80716(266)
C4	.39062(71)	.21558(55)	.71329(284)
C4'	.60321(74)	.21412(56)	.70358(271)
C5	.44277(86)	.28337(56)	.61511(318)
C5'	.55050(82)	.28219(57)	.61810(298)
H1	.32	.205	.56
H2	.402	.326	.54
H1'	.67	.222	.76
H2'	.59	.329	.61

Table IIb

Refined Temperature Factors for TTTI (Lattice 1, c = 3.643 Å)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I	.0494(6)	.0349(5)	.4702(43)	.0020(4)	.0932(13)	-.0075(11)
S	.0465(12)	.0559(12)	.0460(18)	.0180(10)	.0121(12)	-.0006(12)
S'	.0489(12)	.0568(12)	.0449(18)	.0116(10)	.0143(12)	-.0016(13)
C1	.0400(42)	.0523(44)	.0380(59)	.0150(36)	.0061(43)	-.0078(44)
C2	.0476(44)	.0508(43)	.0239(54)	.0145(37)	.0015(41)	-.0072(42)
C2'	.0475(44)	.0528(44)	.0193(51)	.0076(37)	-.0027(40)	-.0082(42)
C3	.0562(49)	.0473(42)	.0158(48)	.0142(38)	-.0033(40)	-.0046(40)
C3'	.0520(47)	.0474(41)	.0253(55)	.0070(37)	.0063(43)	-.0038(42)
C4	.0630(57)	.0540(49)	.0321(59)	.0166(44)	.0018(48)	-.0072(47)
C4'	.0673(56)	.0559(38)	.0194(52)	.0044(44)	.0091(44)	-.0015(44)
C5	.0826(70)	.0461(45)	.0477(76)	.0190(47)	.0090(59)	-.0030(51)
C5'	.0782(67)	.0524(48)	.0314(62)	.0067(47)	.0001(52)	-.0073(48)

	B
H1	8.0
H2	8.0
H1'	8.0
H2'	8.0



Tetrathiotetracene cation in TTTI

(Based on the refinement of Lattice 1, c=3.64 Å)

Thermal ellipsoids are drawn at the 50% probability level

Figure 1

Table III

TTT Geometry in TTTI (Lattice 1, c = 3.643 Å)

Bond Lengths, Å*		Bond Angles*	
C1-C1	1.471(18)	C1-C1-C2	118.5(1.6)°
C3-C3'	1.456(12)	C1-C1-C2'	119.0(1.6)
C5-C5'	1.403(15)	C2'-C1-C2	122.3(8)
C1-C2	1.383(13)	C2'-S'-S	96.3(3)
C1-C2'	1.394(13)	C2-S-S'	95.4(3)
C2-C3	1.414(12)	C1-C2-S	113.1(7)
C2'-C3'	1.396(12)	C3-C2-S	124.2(7)
C3-C4	1.421(13)	C1-C2'-S'	112.7(7)
C3'-C4'	1.416(13)	C3'-C2'-S'	125.3(7)
C4-C5	1.366(14)	C1-C2-C3	122.7(8)
C4'-C5'	1.348(14)	C1-C2'-C3'	122.0(8)
C2-S	1.753(9)	C2-C3-C3'	118.1(8)
C2'-S'	1.742(9)	C2'-C3'-C3	119.5(8)
S-S'	2.075(7)	C2-C3-C4	123.2(8)
		C3'-C3-C4	118.7(8)
H1-C4	0.93	C3-C3'-C4'	116.7(8)
H1'-C4'	0.88	C3-C4-C5	121.3(9)
H2-C5	0.91	C3'-C4'-C5'	122.6(9)
H2'-C5'	0.92	C4-C5-C5'	119.7(1.0)
		C4'-C5'-C5	120.9(1.0)

Direction cosines of the normal to the TTT best plane: 0.0162, 0.2834, 0.9469.

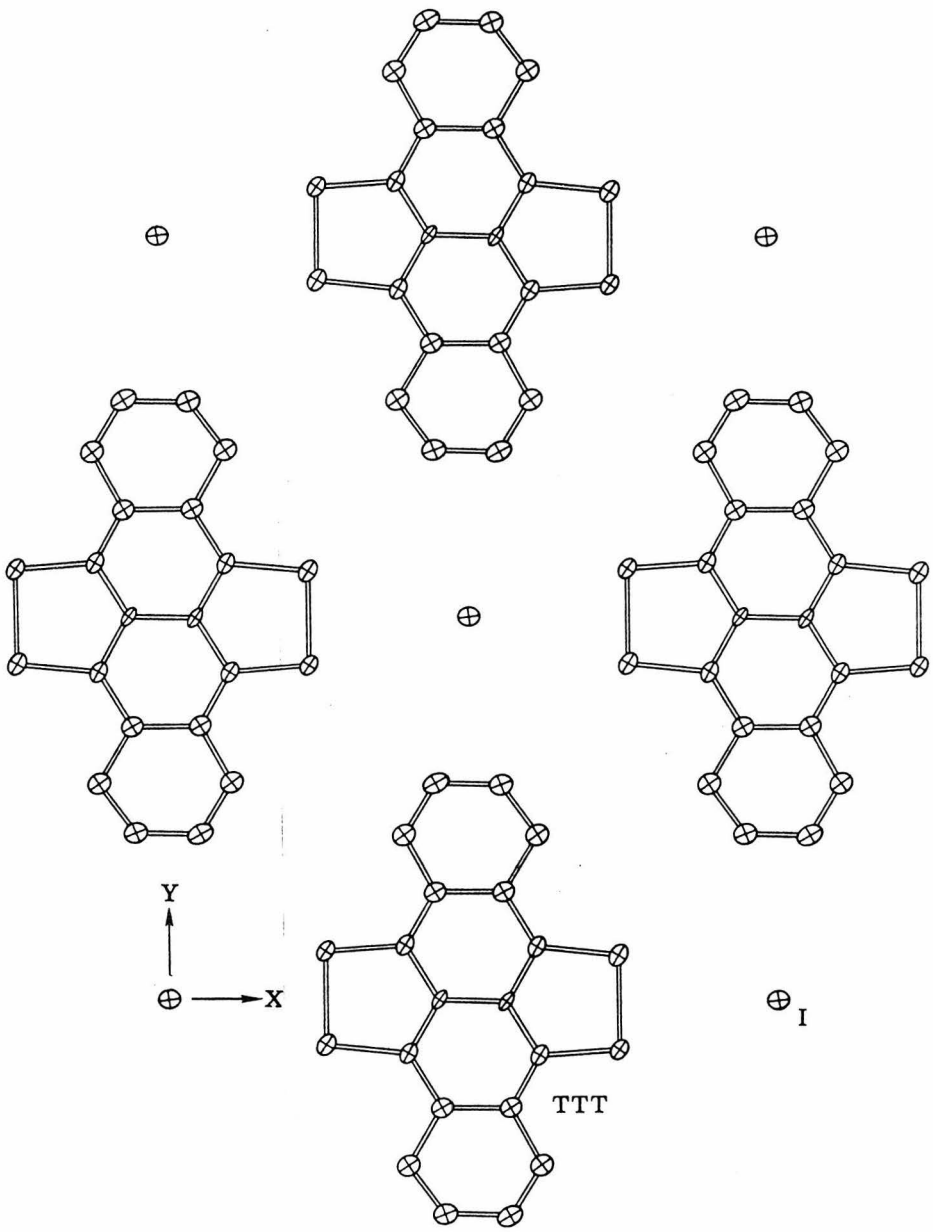
Interplanar distance 3.56 Å.

---

*The numbers in the parentheses are the deviations. The hydrogen atoms were not refined.

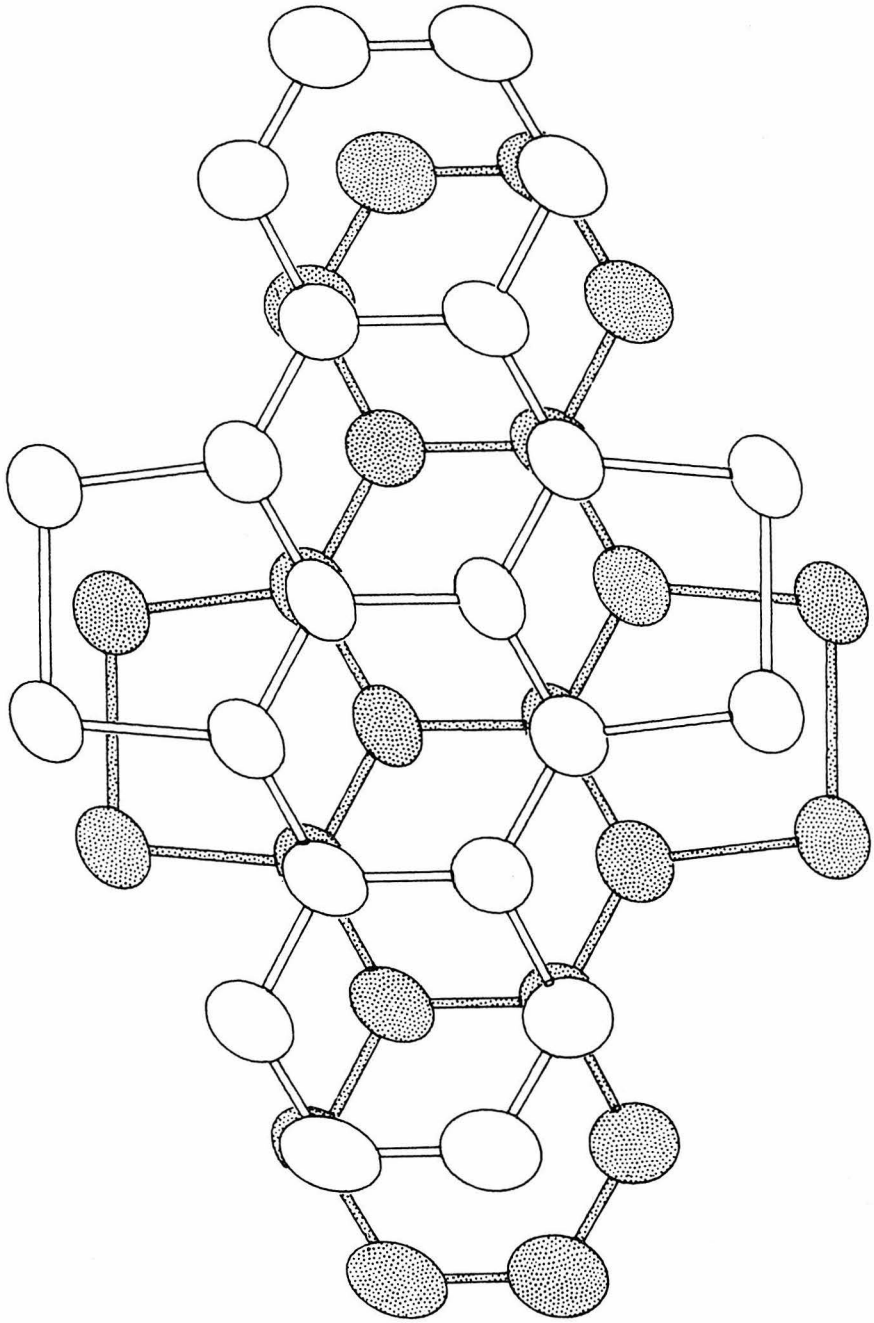
atoms) for the TTT molecule. The TTT molecular geometry is very similar to that of a TTT molecule in TTT_2I_3 (previous Chapter or neutral TTT (8)). However, the arrangement of cation stacks and anion channels is much different in TTTI than in the conducting TTT_2I_3. An [001] projection of TTTI is shown in Figure 2. Whereas in conducting TTT_2I_3 the crystal structure suggests significant interchain coupling, each TTT stack in TTTI is essentially isolated by surrounding iodides from neighboring TTT stacks. There might be only very weak interchain coupling through S-H2 contacts (~3.10 Å) or S'-H2' contacts (~3.04 Å), although these distances are approximately equal to the sum of the van der Waals radii (3.05 Å) (9). The overlap of adjacent TTT molecules in the same stack is also significantly different in TTTI from that of TTT_2I_3. Two adjacent molecules in the same stack viewed perpendicular to the molecular plane are shown in Figure 3. Because there is more overlap in TTTI than in TTT_2I_3 and since the stoichiometry implies a half-filled band, one might expect either a good conductor or a dimerized semiconductor. The transport properties (Appendix B) do suggest semiconductor behavior, but the TTT molecules do not appear to be dimerized. However, the interpretation of transport properties in the presence of two incommensurate lattices is not well understood (10).

As mentioned before the actual crystal structure of this phase consists of two lattices. Shown in Figure 4 is an X-ray oscillation photograph of TTTI rotated about the needle axis, $\vec{c}$, and taken with nickel-filtered copper radiation. In the approximate position of a sixth layer line there are actually two distinct layer lines. Careful



[001] Projection for TTTI

Figure 2

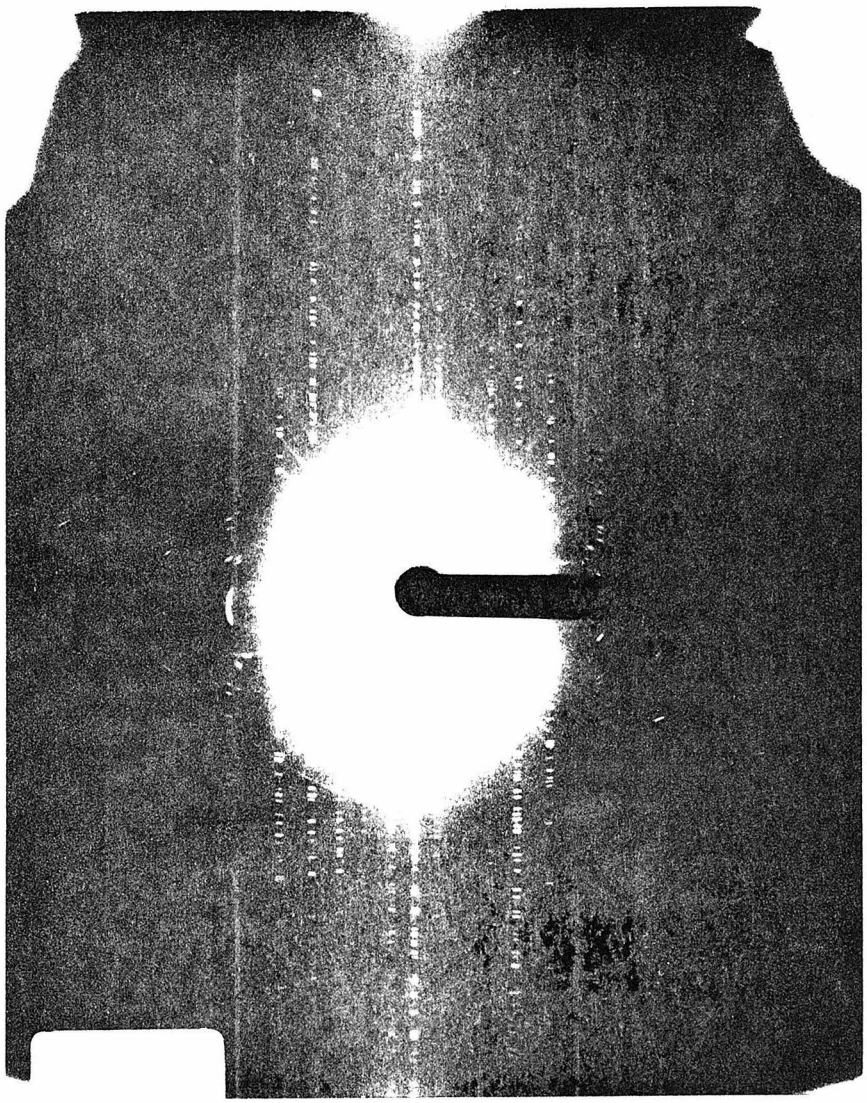


Semiconducting (Tetrathiotetracene)(Iodide), TTTI

Neighboring Tetrathiotetracene molecules, in the same cation stack, viewed perpendicular to the molecular plane.

(Based on the refinement of Lattice 1, c=3.64 Å)

Figure 3



An X-Ray Oscillation Photograph of TTTI (CuK_{α})

Figure 4

measurements of the layer line spacings and the presence of two "sixth" layer lines strongly suggest that a single lattice description of the TTTI structure is inadequate. The layer line spacings obtained from oscillation photographs of two different TTTI crystals are listed in Table IV. These measurements are not absolute, but the measurements for each set of layer line spacings are internally consistent. Although the spacings cannot be fit to a single lattice in the $\vec{c}$ direction, they can be quite adequately fit by assuming the presence of two incommensurate repeat distances in the $\vec{c}$ direction. Structures exhibiting two or more incommensurate lattices are rare, but have been reported (for example 11,12,13). Conceptually TTTI can be viewed as consisting of two structures modulating each other. C. K. Johnson has reported an elegant analysis of the TTF_7I_5 structure, which also consists of two incommensurate lattices (13). Following the indexing method suggested by Johnson, Figure 5 is a graph of the "selection rule" $\ell = 4w + 3t$ where ℓ represents the indexing of an approximate supercell and w and t represent indices of the two sublattices. This graph suggests there might be two layer lines of slightly different spacings for $\ell = 2$ and two layer lines of slightly different spacings for $\ell = 6$. Although two slightly separated layer lines at $\ell = 2$ were not observed, perhaps for lack of intensity, two slightly separated layer lines at $\ell = 6$ were definitely observed. The actual positions of the layer lines can be fit by assuming that planes of spacing 3.642 Å are periodically displaced by an error occuring every 4.787 Å. The period of displacement would occur every Q number of planes (11,14). For

Table IV

Layer Line Spacings of TTTI

Crystal #1	Crystal #2	Interpretation[a]	Calculated Spacings[b]
15.07 Å	15.57 Å	1, $\bar{1}$	15.26 Å
6.86	6.98	$\bar{1}$, 2	6.97
4.75	4.79	0, 1	4.78
3.62	3.65	1, 0	3.64
2.93	2.94	2, $\bar{1}$	2.94
2.458	2.465	3, 2	2.47
2.385	2.391	0, 2	2.39
2.064	2.069	1, 1	2.07
1.822	1.817	2, 0	1.82

[a] $_{w,t}$ w is the index for Lattice 1; t is the index for Lattice 2.

[b] $d = \pm c_1/(|w| \pm |t|/Q)$, $c_1 = 3.642$ Å and $Q = 1.314$.

t \ W	0	+1	+2	+3
0	0	4	8	12
+1	3	7	11	15
−1	−3	1	5	9
+2	6	10	14	18
−2	−6	−2	2	6

W indices for Lattice 1

t indices for Lattice 2

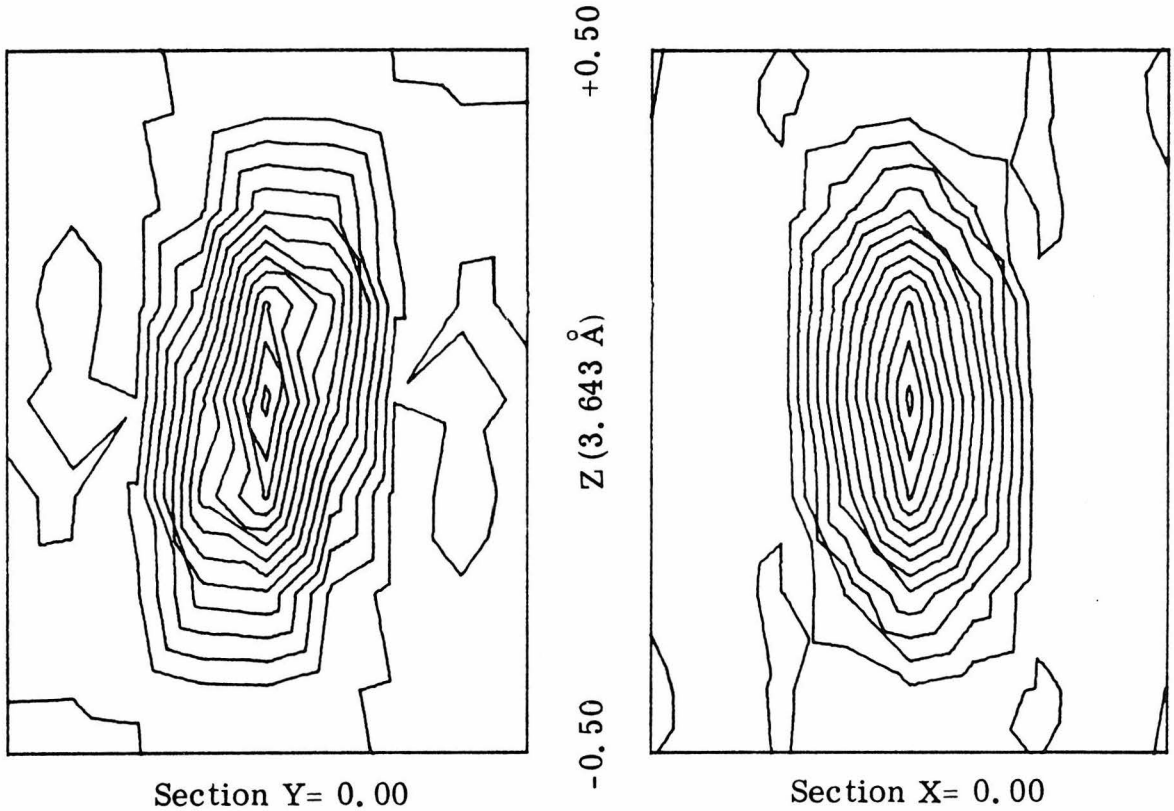
$\ell = 4W + 3t$

Calculations for the indexing of TTTI X-ray Oscillation Photographs

Figure 5

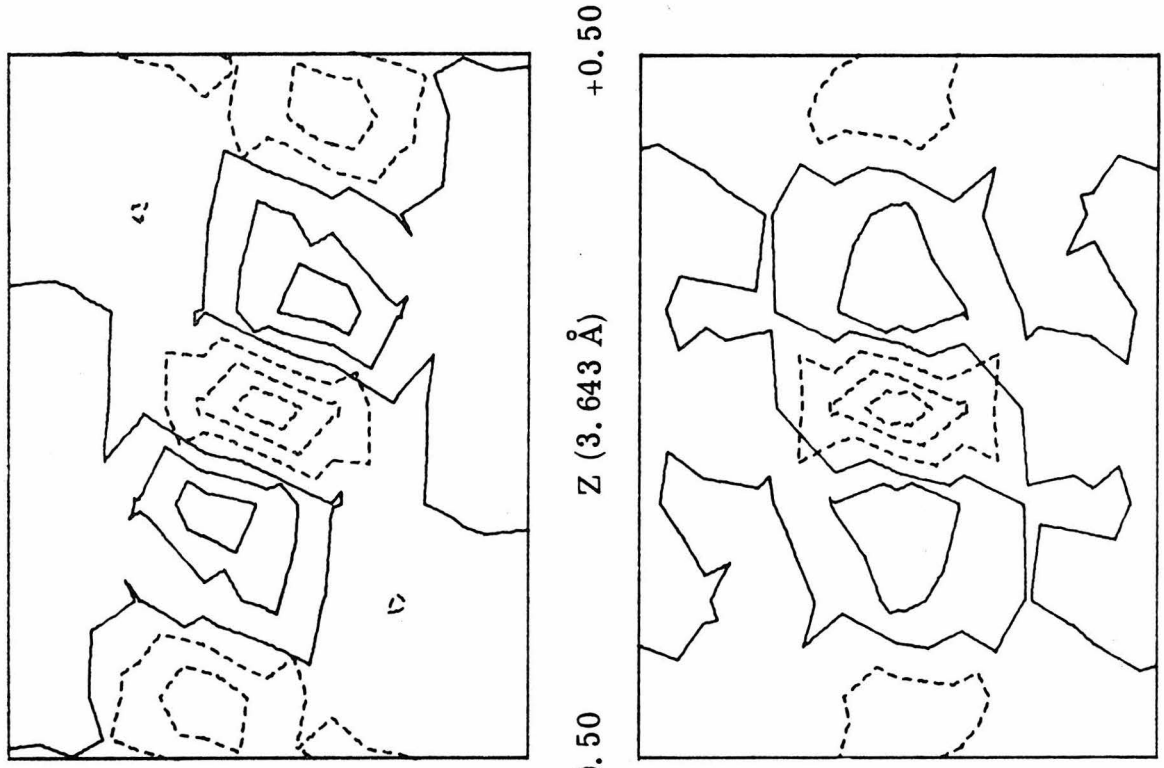
TTTI, Q = 4.787/3.642 = 1.314 planes. If Q equalled a whole number of planes (or a rational fraction), then the periodic error becomes part of the repeat pattern of an exact supercell. For example, if Q = 4 Å/3 Å = 1.3333, then the structure could equally well be described by a supercell with a repeat of 12 Å. In TTTI Q is very far from being a rational fraction. If the periodic displacement is small, James has shown that additional layer lines will be observed at spacings $d = \frac{c_1}{|w| \pm |t|/Q}$ (11,14). James calls the extra lines "ghosts" or satellites, but they could equally well be described as the interference cross terms from the diffraction of two lattices. Shown in the last column of Table IV are the calculated d spacings for TTTI using the w and t indices found from the graph in Figure 5 and based on the values of c_1 = 3.642 Å, c_2 = 4.787 Å, λ = 1.5418 Å ($CuK_{\bar{\alpha}}$). With the exception of the first layer line the agreement is quite good suggesting that TTTI does consist of two lattices incommensurate along $\vec{c}$, but commensurate in a*,b*.

Although only the structure of lattice 1 (c=3.64 Å) has been solved and refined, by analogy to other known channel structures, such as TTF_7I_5 (13), $TTFBr_x$ (15), $TMTSF(SCN)_x$ (16), one can postulate that lattice 2 (c ~4.78 Å) is due to the iodide atoms. This is reasonable considering that refinement of the hk0 projection of both lattices indicated the stoichiometry as TTTI (1:1) which, assuming complete charge-transfer implies I^-. Two times the van der Waals radius of I^- is ~4.3 Å which is intermediate between the lattice spacings 3.64 Å and 4.79 Å. In the lattice 1 structure the iodide is at x = 0, y = 0, z = 0 (Figure 6) but the root-mean-square (rms) displacement along $\vec{c}$ is



TTTI
Electron Density about 0, 0, 0
Contoured at $2e^{-}/Å$ beginning at zero

Figure 6



TTTI

Difference Fourier Sections about 0, 0, 0

——— zero and positive 0.5 e^-/Å contours

------ negative 0.5 e^-/Å contours

Figure 7

approximately 0.69 Å which is about 3.6 times as large as the rms displacement in the other two directions. Difference Fourier sections through the iodide (Figure 7) indicate that positioning the iodide at 0,0,0 in lattice 1 is a reasonable model but the iodide does appear to be at x = 0, y = 0, z ≃ 0.197 occasionally. D_{I-I} for z = 0 to z = 1.197 is about 4.4 Å or the expected van der Waals distance between I^- atoms. This structural determination has shown that:

(A) the crystals have golden reflection and look very similar to TTT_2I_3

(B) this phase is apparently semiconducting

(C) the stoichiometry of this semiconducting phase is TTTI (1:1)

(D) the structure consists of two lattices which are incommensurate along $\vec{c}$, the needle axis of the crystal

(E) the two repeat distances along $\vec{c}$ are c_1 = 3.643(1) Å and c_2 ≃ 4.79 Å.

In 1976 Buravov, et al., (1) reported crystallizing two phases of tetrathiotetracene-iodide. One phase was the highly conducting TTT_2I_3; the other was a semiconducting phase with the reported stoichiometry of TTT_4I_4. Their crystal data for this TTT_4I_4 is listed in Table V. Except for an approximate quadrupling of c_1, their unit cell is the same as TTTI. Although they reported solving the hko projection and were attempting the three-dimensional structure, the only structural information reported was "the existence of parallel stacks of NBDT [TTT] and I along the c-axis is characteristic of the structure" (1). Either Buravov and coworkers did not notice the existence of two incommensurate

Table V

Comparison of the Unit Cell Parameters of TTT_4I_4 and TTTI

TTT_4I_4[a]	TTTI[b]
a = 13.036(2) Å	a = 13.028(2) Å
b = 16.435(2)	b = 16.445(2)
c = 14.582(2)	c = 3.643(1)
α = 90°42'(3)	α = 90.81(1)°
β = 83°49'(3)	β = 96.11(1)
γ = 88°53'(3)	γ = 91.11(1)
Space group, $C\bar{1}$	Space group, $C\bar{1}$

[a]L. I. Buravov, G. I. Zvereva, V. F. Kaminskii, L. P. Rosenberg, M. L. Khidekel, R. P. Shibaeva, I. F. Schegolev, and E. B. Yagubskii, J. Chem. Soc. Chem. Comm., 720 (1976).

[b]This study (Lattice 1, see text).

lattices and used an approximate supercell or they were able to crystallize a semiconducting TTTI with an ordered, single lattice structure. If they did crystallize an ordered, semiconducting TTTI, it would be of interest to know if the TTT molecules were dimerized as would be expected for a static Peierls distortion arising from the half-filled band.

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(7) $R = \sum \left| |F_o| - |F_c| \right| / \sum |F_o|$

goodness-of-fit = $[\sum w(|F_o|^2 - |F_c|^2)^2/(N-P)]^{1/2}$

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Chapter 4

Structure of (Hexamethylenetetraselenofulvalene)(Iodide)$_x$

Hexamethylenetetraselenofulvalene-tetracyanoquinodimethane (HMTSF-TCNQ) is the best organic metal known (1). At 300° K its conductivity is ~2000 Ω^{-1} cm^{-1} and increases with decreasing temperature to about 110° K. Between 45° and 75° K the conductivity goes through a broad maximum and then decreases with decreasing temperature. But the low temperature state appears to be semi-metallic. At 1° K the conductivity is ~600 Ω^{-1} cm^{-1}. Crystals of HMTSF-TCNQ remain conducting to 0.045° K (1). HMTSF-TCNQ is a two charge-carrier system. It would be of interest to synthesize a single-carrier conductor based on HMTSF for comparison with HMTSF-TCNQ.

Experimental

Single crystals of HMTSF-I_x were prepared by R. Williams at Caltech. HMTSF, supplied by Dr. D. Cowan and Dr. P. Shu of Johns Hopkins University, was chemically oxidized to HMTSF$(ClO_4)_x$ by a very dilute solution of H_2O_2 and $HClO_4$ in acetonitrile. Solutions of HMTSF$(ClO_4)_x$ in acetonitrile and tetrabutylammonium iodide in acetonitrile were allowed to slowly diffuse together. Single crystals of HMTSF-I_x grew near the interface.

Two crystalline modifications of HMTSF-I_x were obtained by diffusion. Both crystalline modifications formed dark needles. One modification

formed very poor quality crystals and had a repeat spacing along the needle axis of 10.24 Å. The second modification, the one reported here, formed nice, dark needles. Initial X-ray diffraction photographs showed the crystals to be triclinic with a repeat spacing along the needle axis, $\vec{a}$, of about 8.08 Å

A single crystal with the dimensions 0.396 mm x 0.058 mm x 0.066 mm was chosen for data collection. Based on a least-squares fit of thirty-eight 2θ values obtained with a Syntex $P2_1$ diffractometer the unit cell parameters were determined to be a = 8.056(4) Å, b = 12.740(4) Å, c = 8.016(3) Å, and α = 81.72(4)°, β = 67.73(5)°, γ =102.64(4)° for $\lambda = MoK_{\overline{\alpha}}$ = 0.71069 Å (Table I). The numbers in parentheses represent the estimated standard deviation in the last decimal place. A complete data set to 2θ = 60° was collected on an automated Syntex $P2_1$ diffractometer with monochromatized molybdenum K_α radiation. Intensities were collected with 1° per minute 2θ-θ scans. The time spent collecting background was 50% of the amount of time spent scanning a reflection, or about one minute for each side of a scan. The integrated intensities were corrected for Lorentz and polarization effects. The weights assigned to the reflections and used in the refinement were based on counting statistics. No more than two observations contributed to a weight.

Initial selenium atom coordinates were found from a three-dimensional Patterson map. Preliminary structure factor-Fourier calculations were based on the noncentric space group P1. After most of the atom

Table I

Crystal Data for HMTSF-I_x

a = 8.056(4) Å

b = 12.740(4)

c = 8.016(3)

α = 81.72(4)°

β = 67.73(5)

γ =102.64(4)

V =715.2(9) $Å^3$

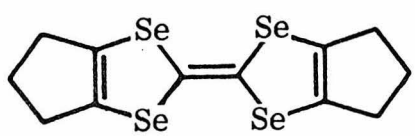
Z = 2

Space group $P\bar{1}$

Linear absorption coefficient (MoK_α), μ = 111.938 cm^{-1} (for the stoichiometry $HMTSF_2I_{0.64}$).

Stoichiometry ~$HMTSF_2I_{0.31}$

Crystal dimensions 0.396 mm x 0.058 mm x 0.066 mm

HMTSF ≡ 

coordinates had been determined and crudely refined, the center of symmetry (inversion center) became obvious. All subsequent calculations were based on the space group $P\bar{1}$. The real parts of the atomic scattering factors of iodine and selenium after correction for anomalous dispersion ($f_0 + \Delta f'$) were used for structure factor calculations (2). There are two HMTSF molecules per unit cell, and they are related to each other by the inversion center. Preliminary least-squares refinement of the structure suggested that the stoichiometry was ~$(HMTSF)_2(I)_{0.64}$/unit cell. Absorption corrections based on this stoichiometry (μ = 111.938 cm^{-1}) were applied to the data set (3,4). Although the crystal used for data collection had six faces parallel to $\vec{a}$, two of the faces were too small to measure. So for the absorption corrections the crystal was approximated as being bounded by the major faces, the (001), (00$\bar{1}$), (010) and (0$\bar{1}$0) faces, and the ends by the (100) and ($\bar{1}$00) planes.

After several full-matrix least-squares refinement cycles the HMTSF molecule was refined but the iodine at 1/2,1/2,1/2 would not converge. Difference Fourier sections about 1/2,1/2,1/2 showed that a single iodine atom at 1/2,1/2,1/2 was a poor description of what was actually present. Further refinement of the structure was accomplished by adjusting the "solvent" atoms, based on the appearance of the difference Fourier sections, followed by a least-squares refinement of all of the HMTSF parameters and the population and temperature factors of the iodine. The "solvent" atoms were assumed

to be approximately equal to carbon in scattering power and were given carbon atomic scattering factors. An unsuccessful attempt was made to find the hydrogen atoms on a low-angle three-dimensional difference Fourier map. The hydrogens have not been included in the structure. The structure was judged to be refined when the R value stopped changing and the difference Fourier map looked reasonable. The final difference Fourier map showed a maximum range of -2.3 e/Å^3 to +2.1 e/Å^3. All shifts in the final least-squares cycle were less than 1/3 σ. For the complete data set of 4209 reflections (3611 reflections had $F_o^2 > 0$) R = 0.098, with a goodness-of-fit of 1.65 (5). For the 2038 reflections with $F_o^2 > 3\sigma (F_o^2)$, R = 0.051. Listed in Table I are crystal data. Listed in Table II are refined atomic coordinates and thermal parameters.

Discussion

One of the primary objectives of a structure determination of a quasi-one-dimensional conductor which contains halide is to determine its stoichiometry. Because one can assume with some confidence that all of the halide present will be as X^-, knowing the amount of X^- in the structure will make the calculation of the number of charge carriers (holes) easy. This is valuable for interpretation of the transport properties. Unfortunately, stoichiometry is the most poorly defined parameter of this structure. The "refined" value of 0.3144 iodines per two HMTSF molecules is, obviously, dependent on the amount

Table IIa

Atomic Coordinates

	X	Y	Z
I	.5	.5	.5
Se1	-.36099(14)	.09124(8)	.20432(12)
Se2	-.18153(14)	.12862(8)	.33786(12)
Se3	-.14371(14)	.05500(8)	-.22328(12)
Se4	.05146(14)	.27062(7)	-.09138(12)
C1	-.19470(116)	.04781(67)	.02878(109)
C2	-.39847(120)	-.14949(66)	.01729(108)
C3	-.52680(143)	-.26156(73)	.04128(134)
C4	-.48679(155)	-.26479(74)	-.16303(131)
C5	-.35653(137)	-.14793(75)	-.29290(124)
C6	-.30915(133)	-.08978(69)	-.16280(118)
C7	-.12495(123)	.13476(71)	.08311(106)
C8	-.03743(122)	.27965(69)	.27695(118)
C9	-.01853(172)	.34484(83)	.41394(137)
C10	.08380(183)	.46475(74)	.28498(143)
C11	.17392(143)	.45430(66)	.07938(133)
C12	.06052(128)	.33674(65)	.09765(113)

Table IIb

Anisotropic Temperature Factors

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I	.0657(35)	.3266(110)	.0459(25)	-.0246(45)	-.0140(23)	-.0092(37)
Se1	.0347(6)	.0274(5)	.0218(4)	.0005(4)	-.0073(4)	-.0004(4)
Se2	.0378(6)	.0248(5)	.0228(4)	.0020(4)	-.0099(4)	-.0022(3)
Se3	.0341(6)	.0251(5)	.0228(4)	.0004(4)	-.0106(4)	-.0005(3)
Se4	.0359(6)	.0246(5)	.0239(4)	.0030(4)	-.0091(4)	.0000(3)
C1	.0255(47)	.0266(41)	.0308(41)	.0053(37)	-.0064(37)	-.0031(33)
C2	.0319(49)	.0260(40)	.0304(40)	.0060(37)	-.0156(38)	-.0055(32)
C3	.0491(63)	.0269(46)	.0474(54)	-.0054(45)	-.0178(49)	-.0068(40)
C4	.0681(75)	.0261(43)	.0431(50)	.0023(48)	-.0273(52)	.0010(37)
C5	.0425(57)	.0307(45)	.0384(47)	.0015(43)	-.0158(43)	-.0057(37)
C6	.0465(58)	.0275(42)	.0379(46)	.0105(41)	-.0230(43)	-.0072(35)
C7	.0315(50)	.0321(45)	.0265(40)	.0060(40)	-.0064(37)	-.0028(33)
C8	.0302(49)	.0309(43)	.0402(46)	.0057(38)	-.0182(40)	-.0101(36)
C9	.0837(85)	.0380(52)	.0452(54)	.0085(56)	-.0350(59)	-.0160(43)
C10	.1027(99)	.0235(44)	.0546(60)	-.0008(56)	-.0350(66)	-.0052(41)
C11	.0513(63)	.0151(38)	.0510(54)	-.0058(41)	-.0198(50)	.0011(36)
C12	.0389(54)	.0225(39)	.0332(41)	.0057(39)	-.0100(40)	-.0020(33)

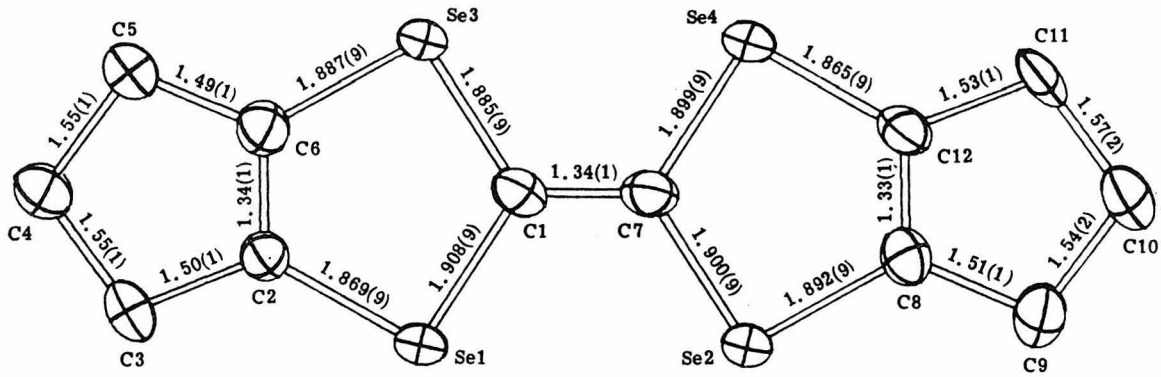
	Population
I	.31443(453)

of "solvent" assumed to be present. By assuming that only iodide or disordered CH_3CN is present, it is reasonable to also put part of a carbon atom at 1/2,1/2,1/2. For 0.39C with a B = 12.0 at 1/2,1/2,1/2, there is also ~0.3144I at 1/2,1/2,1/2. But the actual amount of iodide present could differ from that value by as much as 30%. Another possibility is that the "solvent" is not always CH_3CN but could occasionally be ClO_4^-, which would affect any calculations of the amount of charge transferred. Listed in Table III are the atomic coordinates, populations, and thermal parameters used to model the electron density at and about 1/2,1/2,1/2. The populations and temperature factors are not meaningful and are highly correlated. The temperature factors for the "solvent" atoms were chosen arbitrarily. An attempt was made to use electron microprobe analysis to determine the amount of iodine present in the crystals. Although selenium was found, no iodine was found. Because of the fairly unstable nature of the crystals in solution (6), it was felt that the lack of iodine could be attributed to decomposition of the crystals in the electron beam.

The HMTSF molecule looks quite normal. ORTEP drawings (7) of the HMTSF molecule are shown in Figure 1. There are no significant differences between the HMTSF geometry found in this structure determination and the HMTSF geometry in HMTSF-TCNQ(F_4) (8). Figure 2 is an ORTEP showing the arrangement of HMTSF molecules in one cation stack. The HMTSF molecules slip back and forth much the same as in TMTSF-$Br_{0.82}$ (tetramethyltetraselenofulvalene) (9). The orientation of

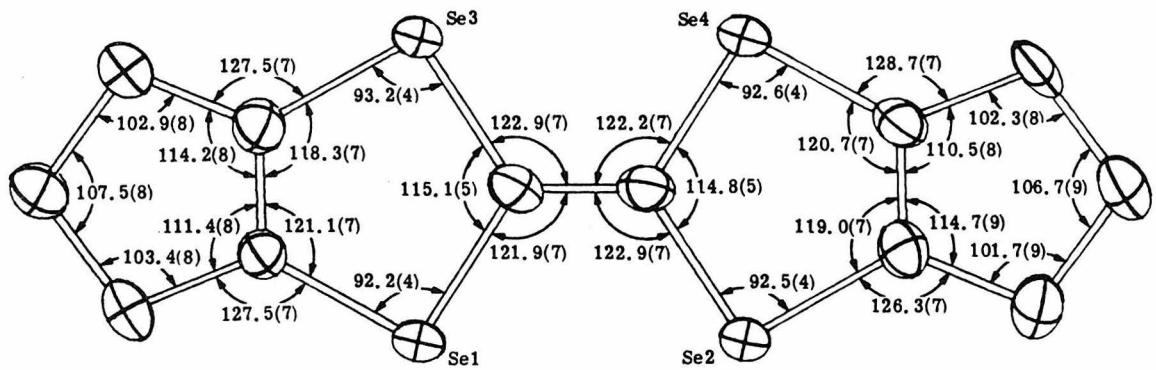
Table III

	X	Y	Z	B	Populations
SOLC	.5	.5	.5	12.0	.39
SOL1	.558	.521	.321	10.0	.33
SOL4	.38	.45	.400	9.0	.25
SOL2	.36	.466	.67	9.0	.33
SOL3	.52	.355	.55	10.0	.32
SOL5	.51	.478	.655	10.0	.17
SOL8	.301	.477	.6	10.0	.20



Bond lengths of HMTSF in HMTSF-I_x (in Ångstroms)

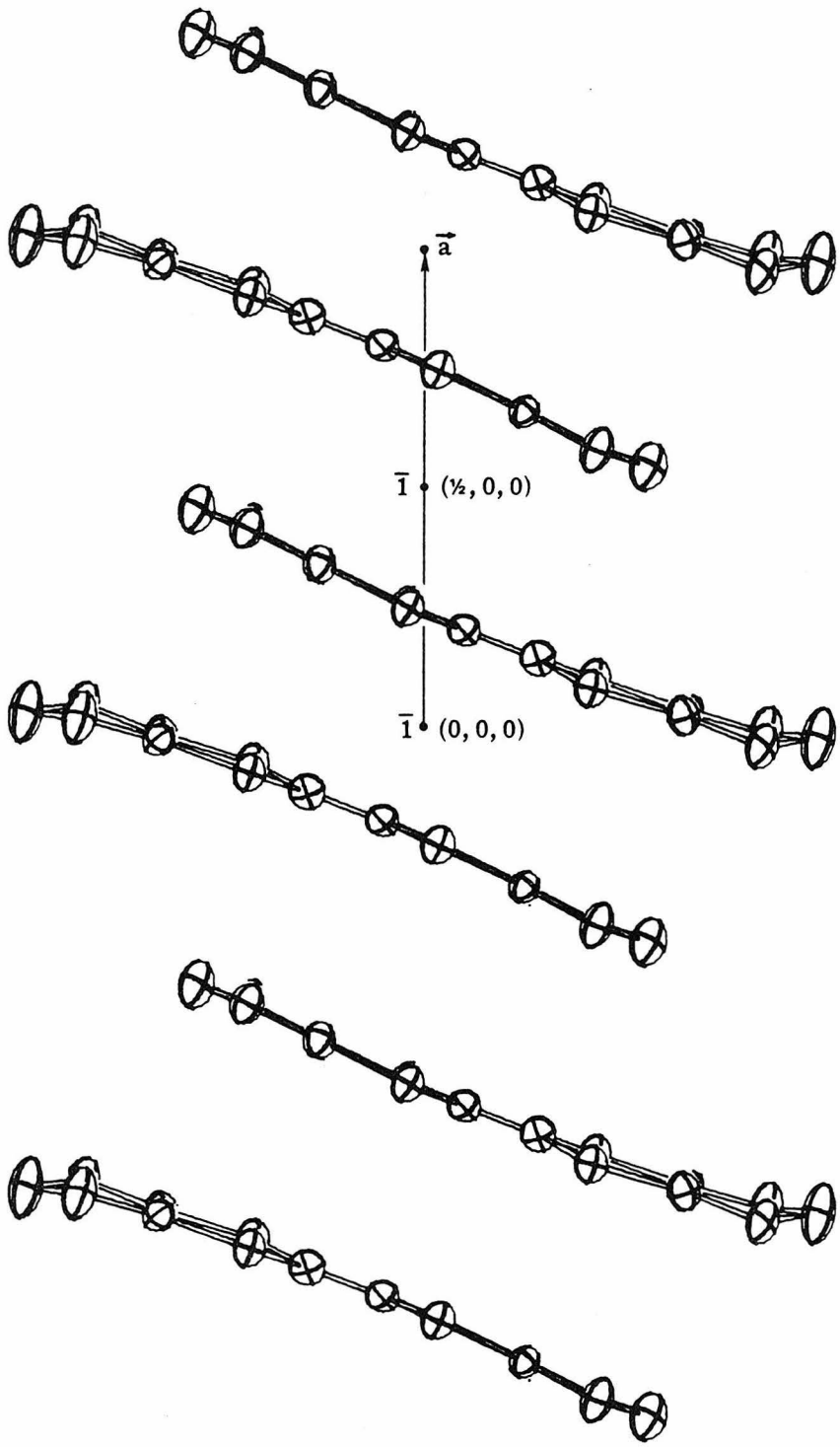
The numbers in parentheses are the estimated standard deviation of the last decimal place.



Bond angles of HMTSF in HMTSF-I_x (in degrees)

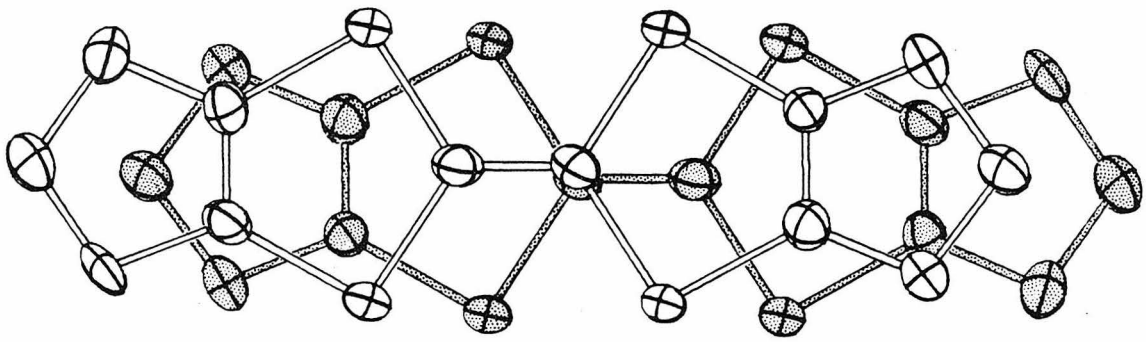
The numbers in parentheses are the estimated standard deviation of the last decimal place.

Figure 1

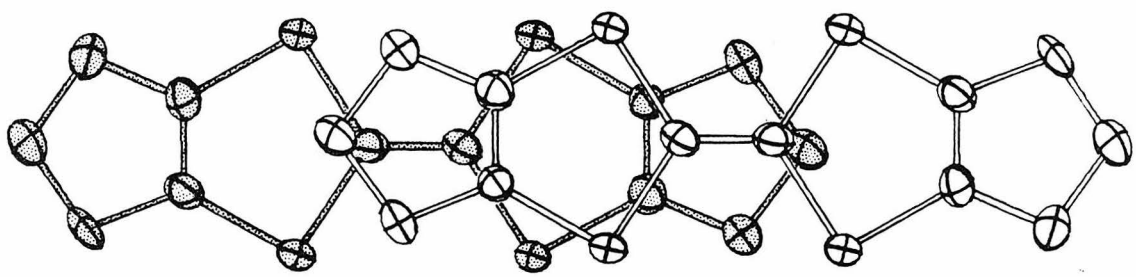


One cation stack along $\vec{a}$ in HMTSF-I_X

Figure 2



Neighboring HMTSF molecules in the same cation stack viewed perpendicular to the molecular plane. The two molecules are related by the inversion center at 0, 0, 0.



Neighboring HMTSF molecules in the same cation stack viewed perpendicular to the molecular planes. The two molecules are related by the inversion center at ½, 0, 0.

Figure 3

neighboring HMTSF molecules, which are in the same cation stack and related by the inversion centers at 0,0,0 and 1/2,0,0, is shown in Figure 3. The amount of slippage of the HMTSF molecules related by the inversion center at 0,0,0 is the same as in TMTSF-$Br_{0.82}$, HMTSF-TCNQ, and other TMTSF, HMTSF, and related structures (for example, 9,10,11,12). However, the neighboring HMTSF molecules related by the inversion center at 1/2,0,0 show a different amount of slippage (See Figure 3).

The room temperature conductivity of HMTSF-I_x is ~1.3-1.7 Ω^{-1} cm^{-1} (13). The temperature-dependence of the conductivity has not been measured. The apparent stoichiometry (1:0.157) certainly suggests that the band formed from overlapping HMTSF orbitals is only partially occupied and that HMTSF-I_x could be metallic. This is reasonable for a tight-binding model, but assumes that the HMTSF molecules are all evenly spaced. However, the HMTSF molecules are not required by the lattice symmetry to be evenly spaced. The results for three least-squares, best plane calculations are listed in Table IV. These results suggest that one cannot unequivocally state that the HMTSF molecules are, or are not, equally spaced. Also influencing the electronic properties of HMTSF-I_x is the presence of a random potential caused by the random occurrence of iodide and "solvent" at 1/2,1/2,1/2. To confirm that there was no superperiod and that the occurrence of iodide and "solvent" was, indeed, random, a very long exposure (92 hours) X-ray oscillation photograph was taken of HMTSF-I_x with nickel-filtered copper K_α radiation. The film was wrapped in aluminum foil to eliminate some

Table IV

Least-square, Best Plane Calculations[a] and Interplanar Spacings for HMTSF-I_x

Plane 1

Atoms	SD[b]	Deviations[c]
Se1	.001	-0.0374
Se2	.001	0.0292
Se3	.001	0.0352
Se4	.001	-0.0435
C1	.009	-0.0070
C7	.0091	0.0235

Direction cosines of the plane normal -0.9226, 0.5698, -0.1827

Interplanar spacings: d_1 = 3.52 d_2 = 3.91 Å

Plane 2

Atoms	SD[b]	Deviations[c]
Se1	.001	-0.0824
Se2	.001	-0.0194
Se3	.001	-0.0069
Se4	.001	-0.0892
C1	.009	-0.0516
C2	.009	0.0498
C6	.010	0.0842
C7	.0091	-0.0226
C8	.0094	0.0941
C12	.0092	0.0440

Direction cosines of the plane normal -0.9230, 0.5692, -0.1840

Interplanar spacings: d_1 = 3.61 d_2 = 3.83 Å

Plane 3

Atoms	SD[b]	Deviations[c]
Se1	.001	-0.1438
Se2	.001	-0.0745
Se3	.001	-0.0471
Se4	.001	-0.1231
C1	.009	-0.1005
C2	.009	-0.0085
C3	.010	-0.0913
C5	.010	0.1586
C6	.010	0.0348
C7	.0091	-0.0690
C8	.0094	0.0483
C9	.010	0.1770
C11	.010	0.0496
C12	.0092	0.0070

(Continued)

Table IV (Continued)

Plane 3 (Continued)

Direction cosines of the plane normal -0.9220, 0.5724, -0.1879

Interplanar spacings: d_1 = 3.70 d_2 = 3.72 Å

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[a]V. Schomaker, J. Waser, R. E. Marsh and G. Bergman, Acta Cryst., 12, 600 (1959).

[b]Coordinate standard deviations from full-matrix least-squares calculation.

[c]Deviations, in Å, from the calculated best plane. All atoms contributed to the best plane with weights of one.

of the longer wavelength fluorescence. There was no indication of any diffuse layer lines or of a supercell.

Figure 3 graphically shows that the overlap between adjacent HMTSF molecules is unique. What a HMTSF molecule "sees" above itself is not the same as what it "sees" underneath itself. This additional potential will cause additional band gaps, although not necessarily at the Fermi surface. Of course, in this HMTSF-I_x structure, since the stoichiometry is ill-defined, the energy of the Fermi surface is equally ill-defined. This structure is the first example of a new type of alternating cation overlap in quasi-one-dimensional conductors.

Because of the subtle interactions of the random potential caused by the disorder at 1/2,1/2,1/2, the band width, the amount of interchain coupling, and the potential from the alternating overlap patterns, a definitive statement about the cause of the apparently semiconducting behavior is difficult to make.

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(5) $R = \sum\left||F_o| - |F_c|\right|/\sum|F_o|$

goodness-of-fit = $[\sum w(|F_o|^2 - |F_c|^2)^2/(N-P)]^{1/2}$

(6) R. Williams, private communication.

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Chapter 5

Summary

The three quasi-one-dimensional conductors studied here have shown a variety of interesting distortions and disorder. Understanding these distortions, disorder, and the overall structures of these materials is important for understanding their physical properties.

Prior to low-temperature structural studies of TTT_2I_3 it was not known whether or not the iodine atoms would order during the phase transitions or whether or not the TTT lattice would undergo a static distortion. For very slow cooling crystals of TTT_2I_3 (h.d.) do not appear to undergo a static distortion. Although all regions of reciprocal space cannot be conveniently sampled with a diffractometer, there was no indication of a major structural phase transition and the iodine chains never achieved long-range three-dimensional ordering. The lack of three-dimensional ordering can be rationalized by assuming the presence of iodides other than I_3^-. I_2 or I^- or other polyiodides will cause static disorder which will not, obviously, be eliminated at low temperatures. This is in contrast to $TTFCl_{.67}$ (1). Because the disorder of the chlorides in $TTFCl_{.67}$ is primarily dynamic disorder, as the temperature is lowered the chloride atoms gradually order and the TTF cations no longer "see" a random potential from the chlorides. With the decrease in the random, screening potential from the chlorides, electrons on the TTF molecules feel the effect of electrons on other

TTF molecules and couple. Coupling allows an overall decrease in the energy of the system. This electronic coupling gives rise to what is described as an electronically driven static Peierl's distortion (2,3,4). With the electronic coupling, a new band gap forms at the Fermi surface and the periodicity of the underlying lattice changes. That change in the lattice has been observed, crystallographically, in $TTFCl_{0.67}$ (1). That a similar effect is not observed in TTT_2I_3 (h.d.) suggests that the static disorder remaining in the iodide chains at low temperatures may cause a random potential sufficient to prevent strong electronic coupling (5). This is consistent with the observation that the phase transitions are most prominent in the crystals with the least disorder (Appendix A).

TTTI is an ordered, quasi-one-dimensional semiconductor which has not dimerized as would be expected for an exactly half-filled band. But since transport properties in crystals with two incommensurate, yet interacting, lattices are not understood, the interpretation of the graphs in Appendix B as being typical of a semiconductor could be incorrect (6).

HMTSF-I_x exhibits an interesting structure. There are primarily five features of the structure which should significantly affect its transport properties. (a) Although the stoichiometry could not be determined accurately from the X-ray data, there are indications that HMTSF-I_x is a non-stoichiometric complex. (b) There are no real "channels" in the structure. The random disorder of iodide and

"solvent" is localized about the coordinates 1/2,1/2,1/2 in the unit cell. (c) The HMTSF molecules may or may not be evenly spaced. (d) Each HMTSF molecule "sees" its two neighbors on either side in the same stack differently. (e) There is probably significant interchain coupling. The magnitude of the conductivity in HMTSF-I_x at room temperature suggests a semiconductor. This is not understood in light of its apparent non-stoichiometry and significant interchain coupling, but the other effects, (b) - (d), could be dominating and those three effects would favor semiconducting behavior.

These iodide-containing structures have shown three different types of iodide behavior in quasi-one-dimensional conductors. In TTT_2I_3 the iodide chains are at least as important, if not more important, than the TTT molecules in determining the observed physical properties. The retention of disorder in the iodide chains at low temperatures has important effects on the low-temperature transport properties. In TTTI the iodides are no longer disordered but are certainly still dominating the structure and causing a modulation of the TTT lattice. In HMTSF-I_x the iodide is probably of minor importance.

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Appendix A

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Effects of disorder on the transport properties of *bis*(tetrathiatetracene)triiodide

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Bis(tetrathiatetracene)triiodide [$(TTT)_2I_3$] is a quasi-one-dimensional organic metal consisting of segregated stacks of tetrathiatetracene (TTT) cation radicals and polyiodide chains. The TTT and iodine (I) sublattices are incommensurate with respect to each other, and the iodine lattice exhibits considerable disorder. In this paper, we report measurements of the conductivity and thermoelectric power of single crystals of TTT_2I_3 in which the degree of disorder is varied. The disorder is modified by crystallization processes and is characterized by x-ray studies. $(TTT)_2I_3$ exhibits metallic behavior at high temperatures ($100°K < T < 300°K$) even in the presence of considerable disorder. Below 100°K, $(TTT)_2I_3$ undergoes a broad metal-nonmetal transition. The effects of disorder on this transition and on the low-temperature transport properties are discussed. The present results are compared with data on $(TTT)_2I_3$ taken by other investigators.

INTRODUCTION

Quasi-one-dimensional organic metals have been the subject of intense interest during the past few years. This interest is due to the many exciting and unusual effects associated with the electronically driven instabilities possible in a one-dimensional electronic system. Most of the organic metals studied have been charge-transfer compounds such as tetrathiafulvalenium-tetracyanoquinodimethanide, TTF-TCNQ, and its derivatives.[1] These compounds have two types of charge carriers with electrons propagating along the acceptor (TCNQ) chain and holes along the donor (TTF) chain. They exhibit metallic behavior down to low temperatures (~60–100 °K), but then undergo a metal-to-nonmetal transition that results in a nonmetallic ground state at $T = 0$ °K. The stabilization of the metallic state and an understanding of the roles of disorder, impurities, and interchain coupling on the metal-to-nonmetal transition have been important goals for many researchers in this field.[1]

In this paper we describe the effects of disorder on the transport properties and metal-to-nonmetal transition in *bis*(tetrathiatetracene)triiodide, $(TTT)_2I_3$. This study is of particular interest for several reasons: (i) In contrast to TTF-TCNQ and its derivatives, $(TTT)_2I_3$ is a single-carrier system with holes propagating along the TTT cation radical stack.[2–4] (ii) $(TTT)_2I_3$ has a high room-temperature conductivity and exhibits metallic behavior down to ~100 °K where a broad metal-to-nonmetal transition commences. Thus the transport properties are quite similar to those observed in the two-carrier systems. (iii) The iodine lattice in $(TTT)_2I_3$ exhibits disorder,[5] and the degree of disorder can be varied somewhat systematically by crystallization processes,[6] therefore, the effects of variable disorder in a given compound may be studied. (iv) Superconducting fluctuations at ~35 ° K have been reported[7] in $(TTT)_2I_3$. It is suggested that the fluctuations are due to one-dimensional effects that become dominant when disorder disrupts the interchain coupling. Our results are compared with those found in other studies of $(TTT)_2I_3$.

SAMPLE PREPARATION AND CHARACTERIZATION

Tetrathiatetracene (TTT) (Fig. 1) was synthesized according to the procedures described by Perez-Albuerne.[8] TTT was recrystallized twice from purified nitrobenzene and subsequently gradient sublimed three times in vacuum. Single crystals of $(TTT)_2I_3$ were obtained by recrystallization from nitrobenzene. TTT and iodine (I_2) were refluxed separately for approximately 1 h in purified nitrobenzene prior to mixing. Upon adding the iodine solution to the TTT solution, the resulting mixture was placed into a temperature bath at ~95 °C. Depending upon the TTT concentration, the mole ratio X of I_2 to TTT, and the cooling rate, single crystals of $(TTT)_2I_3$ with various degrees of disorder in the iodine lattice could be obtained.

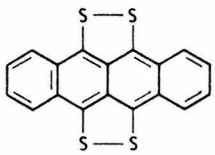

FIG. 1. Molecular structure of tetrathiatetracene (TTT).

Three different kinds of crystals were grown: (a) highly disordered (hd)—crystals with a highly disordered iodine lattice were grown using a TTT concentration of 3×10^{-3} moles/liter, a mole ratio, $X=1.0$, and a cooling rate of 3 °C/h; (b) medium disordered (md)—these crystals were grown with the same concentrations and mole ratio as in (a), but with a slightly faster cool-down rate; and (c) least disordered (ld)—crystals with the least-disordered iodine lattice were grown using a concentration of 5×10^{-4} moles/liter, $X=0.5$, and a cooling period of ~6 days.

The crystals were typically 3–6 mm long and exhibited a brilliant golden reflection. The crystal structures including the disorder of the iodine lattice were studied by x-ray diffraction. Oscillation and Weissenberg photographs were taken at room temperature and at approximately 120 °K, and diffractometer data were obtained at various temperatures ranging from 300 °K to ~27 °K using a low-temperature diffractometer developed locally for this specific purpose.[9] A description of some of the preliminary x-ray results is given in this paper. A detailed report on the crystallographic work will soon be reported.[10]

The room-temperature crystal structure, as determined from diffractometer studies, agrees with that reported by Smith and Luss[5] and by Buravov *et al.*[6] The TTT subcell is orthorhombic with space group *Cmca*, independent of the degree of disorder of the iodine lattice. Figure 2 shows a (010) projection of the crystal structure of $(TTT)_2I_3$. The TTT molecules stack uniformly in a slipped configuration and form segregated chains lying parallel to the *b* axis (the axis of high conductivity). The iodide ions lie in channels situated between the TTT stacks, and also form chains parallel to the *b* axis. Figure 3 shows an oscillation photograph taken at room temperature of a highly-disordered (hd) crystal. It is seen that there are two different sets of layer lines. One set consists of sharp well defined spots (see lines 0, 2, and 4, Fig. 3) associated with the TTT lattice, while the other set is made up of diffuse lines (see 1 and 3, Fig. 3) associated with the iodine lattice. In particular, the diffuseness of the intense third-layer line clearly indicates the presence of disorder. Thus the iodine chains may be slipped relative to one another, along the direction

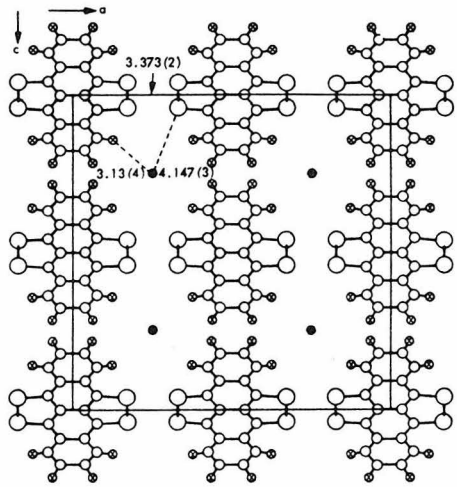

FIG. 2. (010) Projection of the crystal structure of $(TTT)_2I_3$ (from Ref. 5). O—sulfur; ●—iodine; o—carbon; ⊗—hydrogen.

parallel to the stacking axis (*b* axis), such that there is a loss of horizontal registry in the iodine lattice. Oscillation photographs of a medium disordered crystal shows weak spots superimposed on the diffuse third-layer line. These spots are very faint and broad, but indicate that some ordering of the iodine lattice is present, e.g., the iodide chains may be more strongly coupled, resulting in the occurrence of some degree of horizontal registry. In the crystal designated as being least disordered (ld), sharper spots are observed on the diffuse third-layer line. Patterson maps calculated from diffractometer data using $(h3l)$ reflections

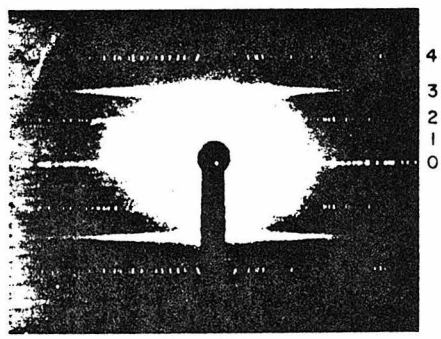

FIG. 3. X-ray oscillation photograph of a highly disordered crystal of $(TTT)_2I_3$ taken at room temperature, using Ni filtered Cu K_α radiation. The numbers label the layer lines.

alone from an ld crystal at room temperature and a hd crystal at 160 °K and 27 °K showed only contributions from the iodide chains. This indicates that the disorder is due solely to the iodide chains and there is little or no contribution to the third-layer line from the TTT subcell. We would like to point out that the ld crystals still exhibit considerable disorder in the iodine lattice. Thus it is believed that small changes in the degree of disorder are being observed.

The classification of the crystals into the three categories, namely, highly disordered, medium disordered, and least disordered, is arbitrary and based on the degree of diffuseness of the third-layer line observed in x-ray oscillation photographs. However, various crystals from the same batch, as well as other batches prepared under the same conditions, exhibit the same degree of diffuseness in the diffraction pattern, and hence we feel that the oscillation photographs provide a useful indicator to estimate the extent of disorder. These conclusions were confirmed by single-crystal diffractometer scans of peak profiles of third-layer spots. The peak profiles of third-layer spots of highly disordered $(TTT)_2I_3$ crystals are very weak, broad, and barely resolvable above the background at room temperature. For the least disordered crystals, the peak profiles are sharper and well resolved on the third-layer line, indicating an increase in the order of the iodine lattice, in agreement with the data obtained from oscillation photographs.

EXPERIMENTAL RESULTS

The electrical conductivity σ along the needle b axis was measured by a standard four-probe technique using aquadag (graphite paint) for electrical contacts. Measurements were made using both dc and ac (16 Hz) techniques. The two types of measurements agreed quite well.

Figure 4 shows the temperature dependence of the normalized conductivity for crystals with different degrees of disorder. Values of the room-temperature conductivity are given in Table I. The conductivity increases with decreasing temperature, as expected for a metal. There is a broad maximum near 100 °K, below which the conductivity decreases with decreasing temperature. Similar temperature dependences for the conductivity have been observed in other quasi-one-dimensional systems.[1,11] Both the peak value of the normalized conductivity $\sigma_p/\sigma_{R.T.}$, and the temperature at which the peak value occurs, T_p^o, decrease

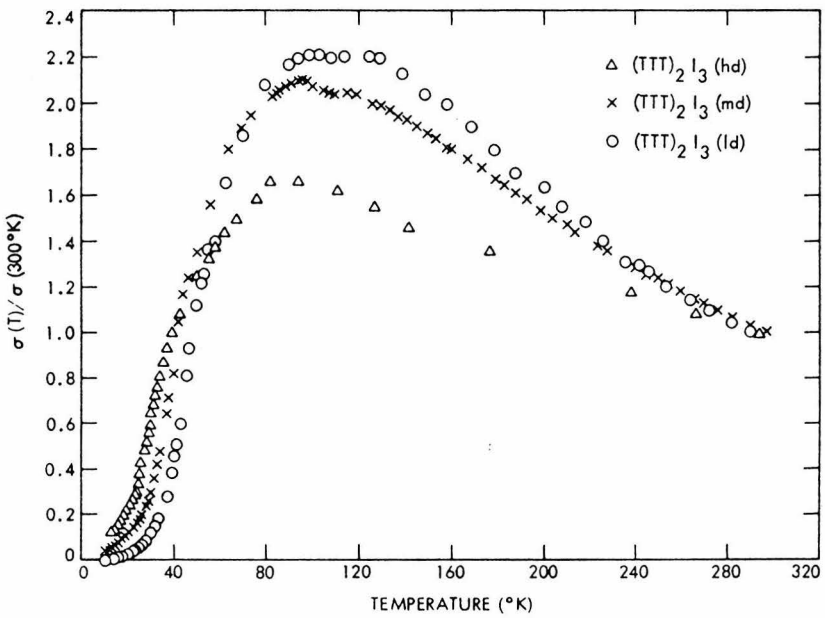

FIG. 4. Temperature dependence of the normalized conductivity of $(TTT)_2I_3$.

TABLE I. Transport parameters of $(TTT)_2I_3$.

$(TTT)_2I_3$	σ_{RT} (Ω^{-1} cm^{-1})	S_{RT} (μV/°K)	σ_p/σ_{RT}	T_ρ^a (°K)	T_{M-I}^a (°K)
highly disordered	1000 ± 250	34 ± 0.2	1.66	82	24 ± 1
medium disordered	850 ± 250	40.7 ± 0.6	2.1	92	~30
least disordered	500 ± 250	42 ± 0.4	2.2	100	35 ± 1

[a] Determined from $d \ln \rho/dT$.

with increasing disorder (see Table I). Figure 5 shows $\ln[\sigma(T)/\sigma(300\,°K)]$ versus reciprocal temperature $1/T$ for the three kinds of crystals. Note that crystals from the same batch agree quite well. The maximum rate of change in slope observed in ld crystals at ~35 °K occurs at lower temperatures with increasing disorder. Measurements of the conductivity,[2,3] ESR linewidth,[3] and high-field magnetoresistance[3,12] of hd crystals have attributed this change to the actual metal-to-nonmetal transition occurring at $T_{M-I} \sim 24$ °K. The other thing to note is that the magnitude of the conductivity at low temperatures e.g., $T \sim 13$ °K, increases with disorder.

The thermoelectric power was measured along the b axis by a technique described in detail elsewhere.[13] The thermoelectric power (S) of several crystals with different degrees of disorder is shown in Fig. 6. The room-temperature values are small and positive for all the samples studied and are shown in Table I. As can be seen, the agreement between samples from the same batch is quite good, and the thermoelectric power (TEP) decreases with decreasing temperature down to ~ 60 °K as expected for hole conduction along a metallic TTT chain. Note that the magnitude and temperature dependence of the TEP in the high-temperature range (300 °K > T >100 °K) does not vary significantly with change in the degree of disorder. Below 60 °K, the thermopower increases in a manner suggestive of nonmetallic behavior.

Another interesting feature is the variation of the peak value of the TEP at 21 °K as a function of disorder. The peak TEP values scales with the degree of ordering and varies from 40 ± 2 μV/°K for the hd crystals to 255 ± 15 μV/°K for the ld samples (see Table II).

DISCUSSION

The crystals of $(TTT)_2I_3$ grown under different crystallization conditions exhibit different degrees of disorder. A room-temperature crystal structure of the ld $(TTT)_2I_3$ using third-level data indicates that the iodine is present in a polyiodide chain with less than full occupancy of all sites.[10] Since there is no well-defined unit such as I_3^-, it seems unreasonable to determine stoichiometry from repeat distances observed in oscillation photographs.

Temperature-dependent x-ray diffraction studies to 27 °K of hd crystals have shown that the iodine chains do not completely order. An oscillation photograph at 120 ± 10 °K of hd crystal was taken after rapidly cooling the crystal in a stream of cold N_2 gas. Beading along the diffuse third-layer line increased in intensity as compared to the room-temperature oscillation photograph. However, Weissenberg photograph ($h3l$) at 120 ± 10 °K showed that there was a significant decrease in normal thermal motion, but the diffuse spots had the same size and shape as at room temperature, indicating residual disorder in the iodine chains and only short-range chain-chain coupling. Thus the apparent intensity gain of the diffuse spots is probably due to a loss of thermal motion, but also, perhaps, to some coalescing of the diffuse background.

Preliminary work on a low-temperature diffractometer[9] to 27 °K indicates that the iodine chains are disordered and minor structural changes may depend on the rate of cooling. Throughout the temperature range studied, the spots on the diffuse third-layer remain quite broad (in the 2θ and ω directions) as compared to normal Bragg reflections from the TTT lattice. The intensities of the broad spots do increase with decreasing temperature. There is no major structural change in the TTT lattice down to 27 °K.

The effect of disorder on the conductivity and the TEP can be discussed best by considering three separate temperature ranges: high temperatures, 300 °K > T > 100 °K, intermediate temperatures, 100 °K > T > 20 °K, and low temperatures, T < 20 °K.

High-temperature region: 300 °K > T > 100 °K

In this temperature range, the conductivity increases with decreasing temperature characteristic of a metal. The resistivity was fitted to

$$\rho(T) = \rho_0 + aT^\gamma, \tag{1}$$

with $\gamma = 2.20$ for crystals with the least disorder. γ decreases to 1.90 for the most highly disordered crystals. This is the trend one would expect since

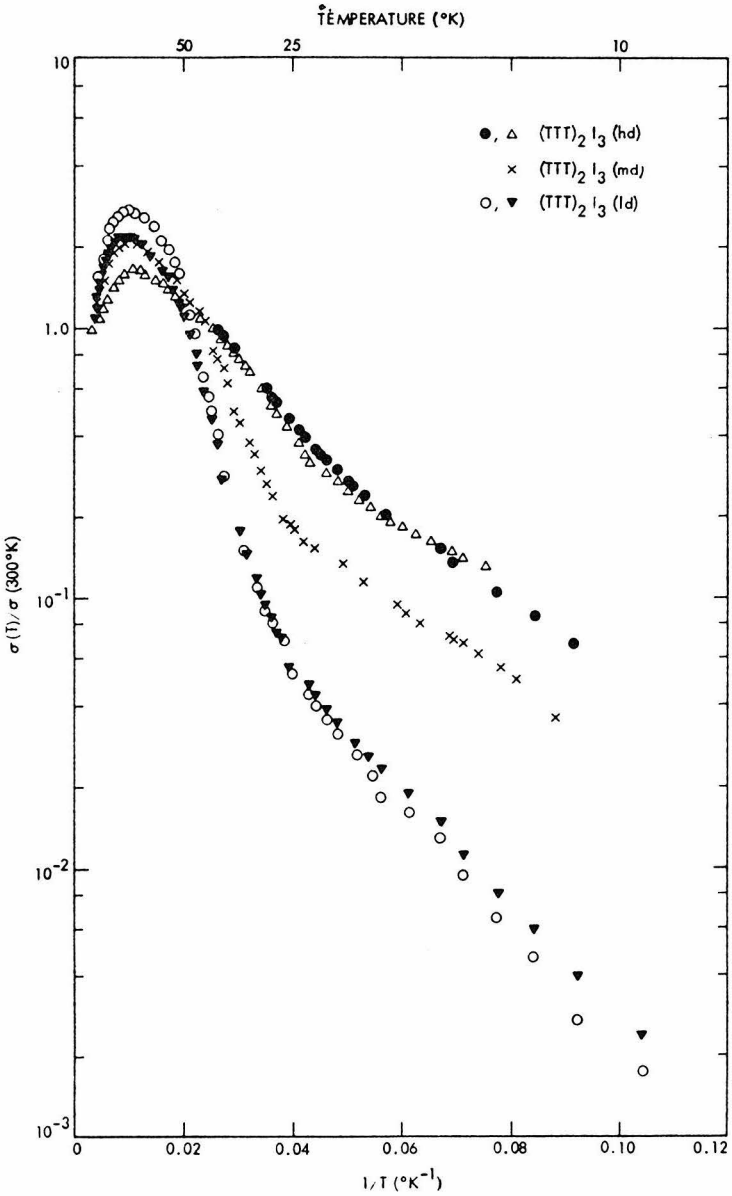

FIG. 5. $\ln[\sigma(T)/\sigma_{RT}]$ vs reciprocal temperature for $(TTT)_2I_3$.

increasing disorder should inhibit metallic transport. The metal-like temperature dependence plus the high value of the room-temperature conductivity suggests that electron transport occurs via delocalized states and that the disorder is not large enough to cause localization at high temperatures. The peak value of the normalized conductivity decreases with increasing disorder. This is similar

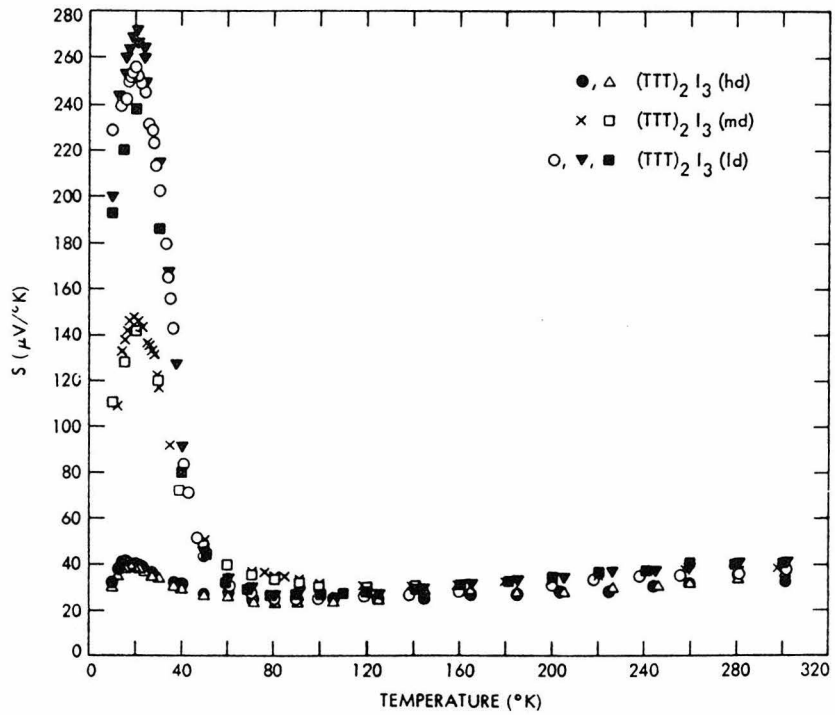

FIG. 6. Thermoelectric power S of $(TTT)_2I_3$.

to what has been observed in TTF-TCNQ, where the disorder was due to excessive thermal cycling[14] or radiation damage.[15] However, in contrast to TTF-TCNQ, the temperature of the conductivity maximum, T_ρ^o, in $(TTT)_2I_3$ does not increase with disorder but shifts to lower temperatures.

TABLE II. Comparison of peak TEP, S_ρ, and normalized low-temperature conductivities, $\sigma(13\,°K)/\sigma_{RT}$, of $(TTT)_2I_3$.

$(TTT)_2I_3$	S_ρ (21 °K) (μV/°K)	$\sigma(13\,°K)/\sigma_{RT}$
JPL		
Least disordered	255	5×10^{-3}
Medium disordered	144	5×10^{-2}
Highly disordered	40	8×10^{-2}
Kodak	40	3.3×10^{-1}
Budapest[a]	20	~0.1
Chernogolovka (Cher.)		
Ordered ($T_\rho^o \sim 110$ °K)	270	...[b]
($T_\rho^o \sim 60$ °K)	110	$\sim 5 \times 10^{-2}$
Most disordered ($T_\rho^o \sim 35$ °K)	~30	...[b]

[a] Unannealed.
[b] Data unavailable.

The TEP of $(TTT)_2I_3$ at high temperatures may be described by a one-dimensional tight binding model. In this case, the thermoelectric power obtained from the Boltzmann equation is

$$S = -(\pi^2 k_B^2 T/6|e|t)[\cos\pi\tfrac{1}{2}\delta/(1-\cos^2\pi\tfrac{1}{2}\delta)], \qquad (2)$$

where t is the transfer integral and δ is the number of conduction electrons per molecule. Although the TEP decreases linearly with decreasing temperature, characteristic of a metal, it does not extrapolate to zero at $T = 0$ °K. This indicates that energy-dependent scattering processes may be important. Nevertheless, the overall linear dependence of the TEP suggests that the room-temperature value and Eq. (2) may be used to obtain an approximate value of the electronic bandwidth, yielding $W = 4t = 0.7$ eV, assuming $\delta = \frac{1}{2}$. This value is consistent with the bandwidth obtained from magnetic susceptibility studies.[2] The temperature dependence of the TEP does not vary significantly with disorder throughout this tem-

perature range. This should be contrasted with the temperature dependence of the conductivity, which does change with increasing disorder. This is what one would expect since the thermoelectric power, unlike the conductivity, is a zero-current measurement and should be less sensitive to disorder.

In summary, $(TTT)_2I_3$ is metallic throughout the temperature range $100\,^\circ K < T < 300\,^\circ K$, even in the presence of observable disorder. This suggests that the rms value of the disorder potential does not dominate the electronic bandwidth.

It is useful to compare the electronic properties of $(TTT)_2I_3$ with those of the halides and pseudohalides of TTF.[16] In both systems, electronic transport is by one carrier only; holes, which propagate along the cation radical chains. Also, there is disorder in the nonconducting anion chains in both types of compounds. While both systems have high room-temperature conductivities and exhibit metallic behavior at high temperatures, the TTF halides and pseudohalides undergo a metal-to-nonmetal transition at relatively high temperatures, i.e., $\sim 200\,^\circ K$, while $(TTT)_2I_3$ remains metallic to below $100\,^\circ K$. We believe that the reason for this different behavior lies in the nature of the stacking of the cation radicals along the chains. In the TTF halides and pseudohalides, the TTF molecules stack in an eclipsed fashion which maximizes the wave-function overlap along the chains and leads to large electronic bandwidths of the order of 1–1.2 eV. In $(TTT)_2I_3$, the TTT molecules are stacked in a slipped fashion which results in smaller bandwidths. Thus $(TTT)_2I_3$ is another example of the empirical trend relating the stability of the metallic state and small electronic bandwidths.[17] This indicates that the more stable metallic state observed in TTF-TCNQ and its derivatives is not critically dependent upon the presence of two different types of conducting chains, and that slipped stacking is favorable for obtaining a more stable metallic state, among other things. Naturally, the nature of the interchain coupling may vary considerably with the type of stacking, with slipped stacking being conducive for the development of significant transverse bandwidth.

Intermediate temperature range: $100\,^\circ K > T > 20\,^\circ K$

Below $100\,^\circ K$, the conductivity decreases with decreasing temperature, indicative of a broad transition from metallic to nonmetallic behavior. With increasing disorder, the change is further smeared out, with the conductivity falling less rapidly with decreasing temperature.

From previous ESR, high-field magnetoresistance and conductivity studies[2,3] of hd $(TTT)_2I_3$, the metal-to-nonmetal transition temperature $T_{M\text{-}I}$ (as determined from the temperature dependence of $d\ln\rho/dT$), is found to be at $\sim 24\,^\circ K$. Thus the region between T_P^o and $T_{M\text{-}I}$ represents a transition region between metallic and semiconducting states which has been broadened by the pronounced disorder. As the disorder diminishes, both T_P^o and $T_{M\text{-}I}$ increase with $T_{M\text{-}I} \sim 35\,^\circ K$ for the ld crystals (see Table II).

The TEP of the least disordered sample attains a minimum value of $\sim 25\ \mu V/^\circ K$ at $\sim 100\,^\circ K$, and then rises steeply to a value of $270\ \mu V/^\circ K$ at $21\,^\circ K$. The TEP always reaches a maximum value at $\sim 21\,^\circ K$, regardless of the degree of disorder. However, the magnitude of the TEP at this temperature decreases with increasing disorder. This, again, indicates that disorder is smearing out the transition and creating states in the single-particle gap.

The TEP in the semiconducting region is very sensitive to the degree of disorder, in contrast to its behavior in the metallic state. Thus the magnitude of the peak value of the TEP at $\sim 21\,^\circ K$ may be used as a rough indicator of the degree of disorder in $(TTT)_2I_3$ compounds. Similar relationships between the magnitude of the peak value of the TEP at low temperatures and the presence of disorder can be found in other quasi-one-dimensional organic metals.[18]

Low-temperature range: $T < 20\,^\circ K$

As seen in Fig. 5, $(TTT)_2I_3$ exhibits a change of slope in the $\ln\sigma/\sigma_{RT}$ vs $1/T$ plot at about $\sim 24\,^\circ K$ in ld crystals. With increasing disorder, the slope in the low-temperature side decreases significantly. Also, the change in slope is less evident in the hd crystals. We believe that these facts indicate that below $\sim 24\,^\circ K$, $(TTT)_2I_3$ is a disordered semiconductor. Conductivity studies to very low temperatures (~ 100 mK) are in progress in order to further elucidate the conduction processes in the nonmetallic state. As the disorder increases, states are formed in the gap resulting in a reduced effective gap and an increased conductivity at low temperatures. Since the value of the conductivity at low temperatures, e.g., $13\,^\circ K$, appears to vary considerably with disorder, we feel that it (as well as the peak TEP) may serve as a rough indicator of the degree of disorder in the crystal (see Table II).

$(TTT)_2I_3$ has been the subject of several previous studies.[2-6] Since the results of Kaminski *et al.*[6] (Chernogolovka. Lab) are quite unusual and different from the results of Isett *et al.*[2] (Kodal Lab), Mihaly *et al.*[4] (Budapest Lab), Somoano *et al.*[3] [Jet

Propulsion Laboratory (JPL)], and those discussed in this paper, it is useful to make a more detailed comparison. It has been shown that $(TTT)_2I_3$ can form crystals with varying degree of disorder in the iodine lattice. Comparing the properties of samples prepared by different groups, therefore, involves an assignment of the relative amount of disorder. As has been suggested earlier in this paper, rough indicators of the disorder are the magnitudes of the low-temperature conductivity and the peak value of the TEP at ~ 21 °K.

The values of the normalized conductivity at ~ 13 °K and the peak values of the TEP for samples from various laboratories are shown in Table II. These two indicators suggest that the Budapest samples are the most disordered. The Kodak samples are similar to our hd samples. X-ray data on the Kodak samples[5] support this conclusion, since no diffuse spots are seen on the third-layer lines of oscillation photographs of these crystals. In addition, derivative analysis[2] of the Kodak conductivity data reveals a transition at $T_{M\text{-}I} \sim 21$ °K.

The degree of ordering of the Chernogolovka samples is obtained from the work of Kaminski *et al.*,[6] and the samples are labeled by their values of T_ρ^o. Comparison with these samples is difficult since the values of σ (13 °K)/σ_{RT} are known for only one sample. Nevertheless, a comparison does offer some insight. The most ordered sample from the Chernogolovka. Lab gives a peak TEP value in good agreement with our ld sample. As the disorder increases, the conductivity peaks of the Chernogolovka samples sharpen up and both T_ρ^o and $T_{M\text{-}I}$ decrease. In addition, the conductivity continues to increase in a metallic fashion with increasing disorder to yield high values of σ_ρ/σ_{RT} 9. This behavior is quite different from that found in the JPL, Kodak, and Budapest samples. The dominant effect of disorder in the latter samples is to smear the transition from the metallic to the semiconducting state and to decrease T_ρ^o and $T_{M\text{-}I}$. Disorder inhibits metallic transport but enhances the low-temperature conductivity in the semiconducting state by providing states near the Fermi level in the single-particle gap. It is important to stress that x-ray studies of the JPL samples at 27 °K indicate that structural disorder is still present. The dominant effect of disorder in the Chernogolovka samples is to decrease T_ρ^o and $T_{M\text{-}I}$ only.

The reason for the difference between the properties of the Chernogolovka samples and those from other laboratories is presently unknown. However, we believe that a significant factor is the tendency of the iodine lattice to order at low temperatures in the Chernogolovka samples. This effect was observed in recent x-ray diffuse scattering studies of the highly disordered Chernogolovka samples by Comés.[19] It is not known whether the ordering of the iodine lattice occurs gradually or discontinuously, and the actual degree of ordering is unknown. Nevertheless, electron scattering by disorder should decrease at low temperatures, thus allowing large values of the conductivity (and, hence, σ_ρ/σ_{RT}) to be attained prior to $T_{M\text{-}I}$. An obvious question associated with this point is: why doesn't the iodine lattice of the JPL, Kodak, and Budapest samples show signs of significant ordering? At present, the answer is unknown. Slight differences in the exact nature of the disorder, the presence of impurities, subtle differences in the interchain coupling, and differences in the amount of excess iodine between the Chernogolovka Lab samples and ours could contribute to differences in the tendency to order. This occurrence of low-temperature ordering is at variance with the model suggested by Abrahams *et al.*[7] They suggest that the disorder disrupts the interchain coupling making the system more one dimensional such that superconducting fluctuations at ~ 35 °K occur. This suggestion may be premature. It should be stressed that the occurrence of ordering in the iodine lattice at low temperatures does not provide a single consistent explanation of the differences observed in $(TTT)_2I_3$ in different laboratories. However, we feel that this feature will play a prominant role in any eventual model that consistently explains the overall behavior of $(TTT)_2I_3$. Obviously, additional low-temperature structural studies would be quite valuable.

CONCLUSIONS

Crystals of $(TTT)_2I_3$ have been grown using different crystallization parameters to yield samples with varying degrees of disorder in the iodine lattice. $(TTT)_2I_3$ is metallic at high temperatures ($T > 100$ °K), even in the presence of observable disorder. A metal-to-nonmetal transition occurs at $T_{M\text{-}I} \sim 24$–35 °K. The effects of disorder are to: (i) reduce the maximum in the conductivity at high temperatures, (ii) broaden the metal-to-nonmetal transition over a large temperature range, (iii) decrease the metal-to-nonmetal transition temperature $T_{M\text{-}I}$, and (iv) enhance the conductivity in the nonmetallic state. In particular, the low-temperature conductivity and thermoelectric power are rough indicators of the degree of disorder. A comparison of measurements made on $(TTT)_2I_3$ at different laboratories indicates that tendencies for the iodine lattice to order at low temperatures may lead to the very different behavior observed in the conductivity by different researchers.

ACKNOWLEDGMENTS

We wish to acknowledge useful discussions with L. Isett, A. Rembaum, and R. Comés. Thanks are due to Mehry Askarian for technical assistance and D. L. Smith for permission to reproduce one of his figures. Part of this work represents one phase of research performed by the Jet Propulsion Laboratory and the California Institute of Technology, sponsored by the National Aeronautics and Space Administration, Contract NAS7-100. A portion of the x-ray crystallographic studies, especially the development of the low-temperature x-ray goniometer, was sponsored by the NSF under Grant No. DMR74-19029A1 (Contribution No. 5958). P. M. C., an A. P. Sloan Foundation Fellow, acknowledges research support by the NSF under Grant No. DMR76-83421.

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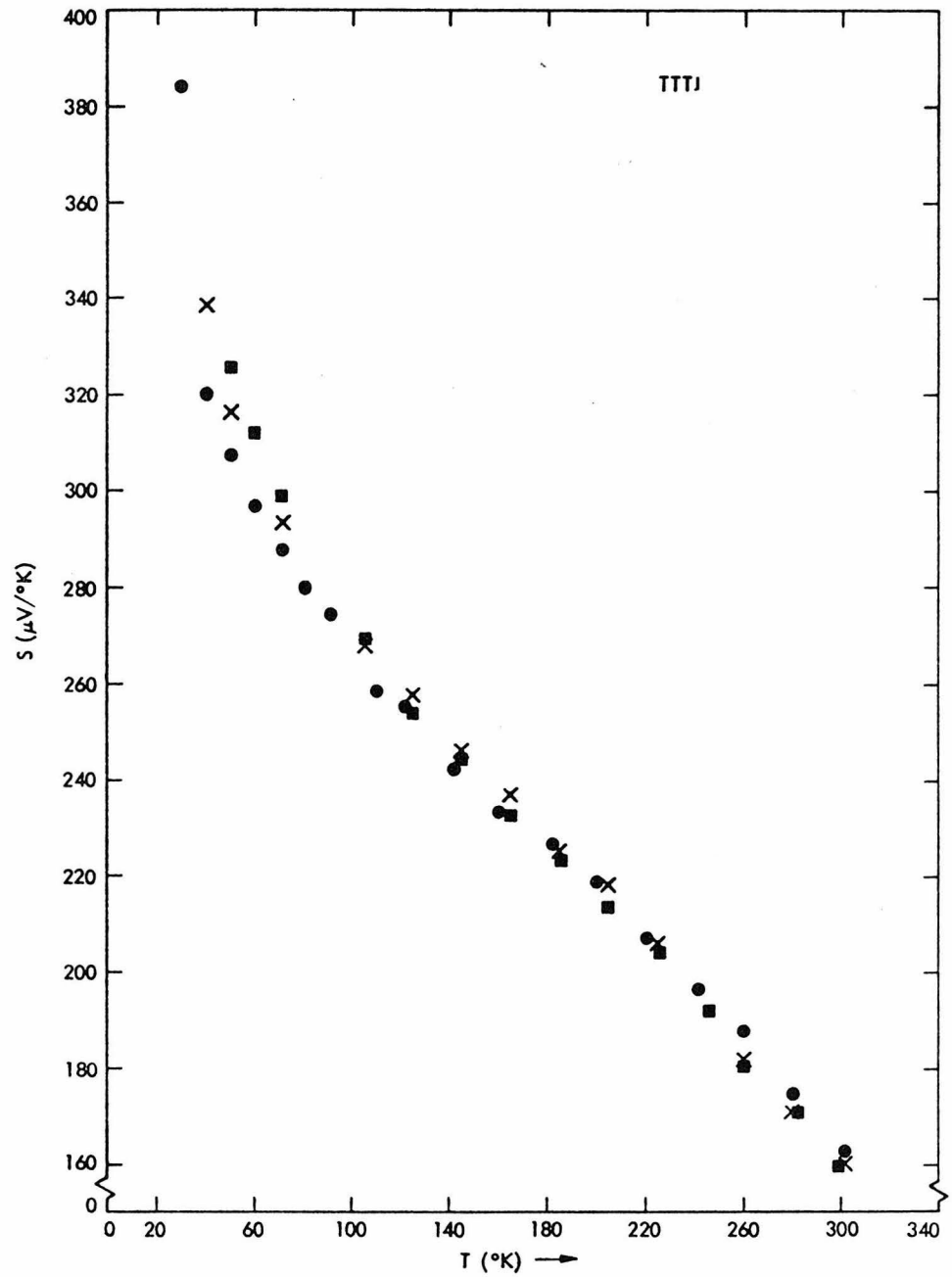
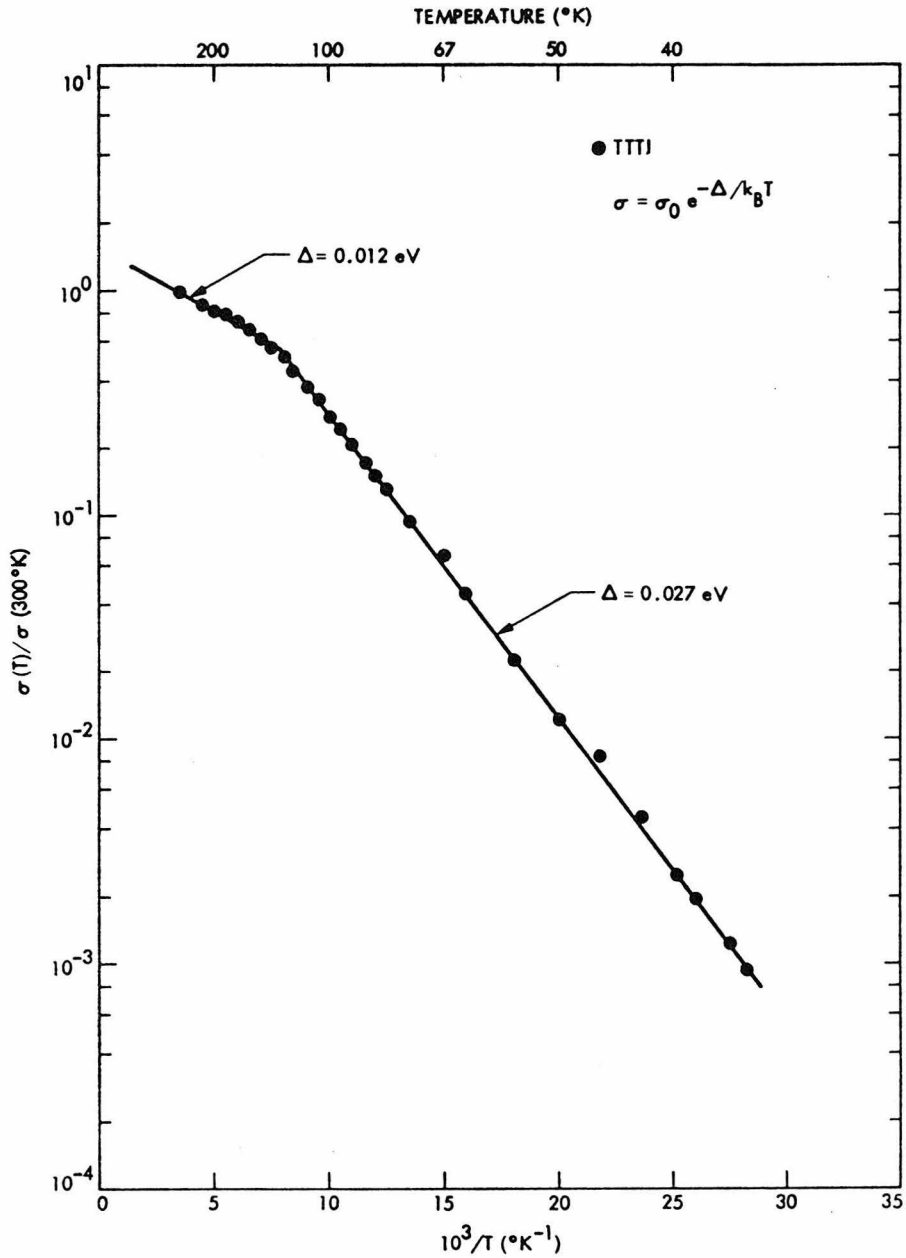
Appendix B

Conductivity and Thermoelectric Power Measurements of (Tetrathiotetracene)(Iodide)

Two graphs are shown for the conductivity and thermoelectric power of TTTI as functions of temperature. The measurements were made by R. B. Somoano and S. K. Khanna at the Jet Propulsion Laboratory.


TTTJ
S (μV/°K)
T (°K) →
400
380
360
340
320
300
280
260
240
220
200
180
160
0
0
20
60
100
140
180
220
260
300
340


TEMPERATURE (°K)
200
100
67
50
40
TTTJ
$\sigma = \sigma_0 e^{-\Delta/k_B T}$
Δ = 0.012 eV
Δ = 0.027 eV
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
σ (T)/σ (300°K)
0
5
10
15
20
25
30
35
$10^3/T$ (°K^{-1})

Appendix C

Observed and Calculated Structure Factors

The following pages list the observed and calculated structure factors for the room-temperature, 164° K, 74° K, and 19° K (Cmca) structures of TTT_2I_3 (h.d.), for TTTI, and for HMTSF-I_x. For each hkℓ the numbers from left to right are $10|F_o|$, $10|F_c|$, and $10(F_o^2-F_c^2)/\sigma(F_o^2)$.

TTT213 (H.D.) ROOM TEMP. COPPER PAGE 1

0 0 L

2	382	217	370
4	2850	2968	-50
6	1705	1546	76
8	1340	1207	127
10	2337	2365	-14
12	501	445	103
14	1654	1671	-14
16	398	400	-3
18	698	699	-1
20	428	429	-2
22	291	287	10

2 0 L

0	1469	1074	213
2	2062	2117	-27
4	3146	3560	-96
6	2414	2375	13
8	1821	1716	77
10	2091	2067	14
12	518	469	97
14	1183	1192	-9
16	462	459	6
18	556	567	-20
20	381	392	-24
22	474	518	-95

4 0 L

0	2108	2043	29
2	2838	3272	-177
4	1935	1927	3
6	1999	1959	25
8	1736	1689	36
10	703	657	77
12	1964	1948	10
14	699	679	32
16	777	779	-3
18	414	417	-6
20	299	319	-49
22	221	236	-42

6 0 L

0	1541	1452	53
2	3162	3400	-84
4	1002	897	130
6	1890	1857	24
8	2051	2027	14
10	1092	997	106
12	1359	1323	35
14	258	223	72
16	995	1002	-8
18	444	428	33
20	313	331	-44
22	194	212	-48

8 0 L

0	332	287	97
2	2784	3010	-118
4	1413	1333	72
6	1766	1763	2
8	1662	1636	21
10	629	542	143
12	1527	1464	53
14	376	363	27
16	776	782	-9
18	301	302	-2
20	252	272	-52

10 0 L

0	2289	2492	-113
2	1168	1149	21
4	1526	1505	17
6	1315	1210	99
8	1042	946	111
10	982	918	76
12	1030	970	69
14	892	769	46
16	427	411	33
18	370	380	-23
20	281	309	-81

12 0 L

0	1946	2116	-116
2	385	314	156
4	1642	1691	-41
6	1029	1010	23
8	801	737	90
10	1829	1751	58
12	475	393	141
14	1024	958	76
16	228	244	-40
18	422	460	-92

14 0 L

0	1601	1706	-92
2	435	399	79
4	1289	1321	-33
6	764	773	-14
8	558	537	38
10	620	594	44
12	644	656	-20
14	768	755	19
16	135	166	-87
18	276	304	-91

16 0 L

0	552	534	32
2	846	870	-36
4	687	693	-10
6	663	658	8
8	672	655	19
10	664	640	26
12	321	327	-15
14	314	331	-48
16	259	293	-119

18 0 L

0	250	268	-46
2	946	943	4
4	247	237	26
6	539	534	10
8	621	640	-36
10	172	173	-2
12	567	573	-12
14	68	92	-74

20 0 L

0	168	160	21
2	874	868	8
4	187	187	0
6	449	449	0
8	451	456	-11
10	78	31	77

22 0 L

0	262	265	-10
2	334	333	2
4	280	278	6
6	285	283	6

1 1 L

1	295	324	-59
2	338	336	3
3	1521	1533	-7
4	2104	2142	-17
5	1172	1136	28
6	914	912	2
7	143	137	17
8	167	175	-24
9	238	242	-12
10	437	437	0
11	173	172	2
12	35	9	12
13	226	223	7
14	-24	10	-5
15	150	150	0
16	104	85	27
17	150	150	0
18	453	453	0
19	240	246	-14
20	210	220	-23
21	21	43	-14
22	13	5	1
23	-12	15	-6

3 1 L

TTT213 (H.D.) ROOM TEMP. COPPER PAGE 2

1	1093	1154	-52
2	709	790	-101
3	382	438	-105
4	360	427	-133
5	137	115	57
6	1302	1360	-61
7	477	437	89
8	1276	1258	17
9	462	474	-28
10	449	427	50
11	444	446	-4
12	206	202	10
13	392	389	7
14	185	176	18
15	414	402	26
16	407	405	4
17	228	237	-20
18	112	105	10
19	108	110	-3
20	170	161	20
21	82	75	11
22	148	157	-23

5 1 L

1	735	726	9
2	319	346	-40
3	76	125	-92
4	471	522	-123
5	161	141	51
6	202	243	-128
7	351	351	0
8	172	208	-104
9	60	3	34
10	407	391	36
11	471	429	87
12	57	53	3
13	113	133	-34
14	75	56	19
15	25	18	2
16	40	34	3
17	-41	4	-12
18	120	103	27
19	97	97	0
20	128	125	5
21	24	46	-16
22	53	52	1

7 1 L

1	309	315	-15
2	92	118	-39
3	196	204	-18
4	147	145	4
5	251	228	32
6	75	63	15
7	298	277	52
8	159	172	-30
9	73	55	19
10	111	93	26
11	162	165	-6
12	88	63	24
13	111	74	42
14	-31	13	-8
15	133	122	17
16	52	65	-10
17	100	107	-9
18	-13	30	-8
19	88	103	-24
20	9	9	0
21	39	2	20

9 1 L

1	614	659	-87
2	452	474	-50
3	776	782	-9
4	1198	1206	-8
5	413	417	-8
6	844	869	-36
7	42	3	13
8	593	583	18
9	348	316	67
10	424	422	4
11	295	308	-28
12	144	139	7
13	428	403	48
14	116	110	8
15	126	135	-14
16	153	144	16
17	56	21	21
18	366	360	13
19	133	137	-8
20	203	217	-40
21	24	21	2

11 1 L

1	428	459	-74
2	278	305	-60
3	299	311	-31
4	282	306	-60
5	87	81	6
6	717	724	-11
7	278	302	-52
8	819	774	62
9	432	388	83
10	223	207	28
11	90	120	-34
12	164	145	28
13	367	316	97
14	190	176	23
15	302	286	34
16	308	290	39
17	245	230	35
18	126	124	4
19	30	9	13
20	48	50	-3

13 1 L

1	78	80	-2
2	112	109	5
3	64	83	-24
4	45	51	-4
5	56	63	-6
6	442	455	-27
7	427	435	-17
8	372	376	-8
9	140	156	-30
10	49	54	-3
11	61	26	22
12	28	18	3
13	70	67	3
14	142	128	26
15	296	297	-2
16	290	302	-31
17	42	54	-15
18	-17	17	-10

15 1 L

1	403	416	-30
2	265	283	-47
3	240	257	-43
4	480	493	-28
5	266	247	45
6	349	352	-7
7	103	123	-36
8	215	214	2
9	36	51	-11
10	315	294	48
11	354	323	71
12	24	28	-1
13	80	80	0
14	56	43	16
15	59	31	34
16	35	27	8
17	46	53	-14

17 1 L

1	302	307	-13
2	169	172	-7
3	114	123	-17
4	211	217	-15
5	57	31	22
6	372	367	12
7	126	112	28
8	320	315	12
9	75	77	-3
10	219	207	32
11	241	221	56
12	64	59	7
13	127	137	-30
14	38	27	13
15	157	167	-38

19 1 L

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	34	14	12
	40	17	16
	75	92	-31
	60	66	-9
	87	90	-5
	105	106	-2
	106	99	16
	38	44	-6
	-18	11	-6
	40	40	0
	25	9	10
	11	11	0

21 1 L

	199	198	3
	139	143	-12
	201	194	23
	282	277	15
	-27	22	-20
	344	339	14
	90	99	-28
	308	305	9
	160	171	-43

0 2 L

0	1064	1179	-150
1	321	307	38
2	238	224	40
3	1202	1137	71
4	927	885	57
5	880	864	23
6	364	343	53
7	1742	1683	28
8	606	535	129
9	1236	1192	45
10	653	634	33
11	448	454	-13
12	126	116	20
13	449	440	18
14	865	855	14
15	474	482	-18
16	104	134	-56
17	358	361	-7
18	112	82	51
19	187	174	35
20	33	32	0
21	222	231	-28
22	27	37	-12

2 2 L

0	597	578	33
1	43	0	19
2	86	5	88
3	810	824	-22
4	672	683	-21
5	594	583	22
6	367	373	-17
7	317	331	-42
8	928	887	56
9	170	145	65
10	280	264	46
11	257	249	22
12	99	65	51
13	120	124	-7
14	68	60	8
15	153	158	-11
16	176	156	45
17	223	213	25
18	214	196	47
19	177	175	5
20	177	173	11
21	111	115	-10
22	22	57	-45

4 2 L

0	444	456	-27
1	539	508	60
2	904	977	-108
3	556	568	-26
4	115	48	71
5	699	699	0
6	307	329	-48
7	140	132	14
8	282	278	8
9	381	361	35
10	254	238	29
11	16	25	-2
12	366	336	52
13	59	60	0
14	194	185	15
15	118	113	6
16	241	216	46
17	101	99	2
18	151	127	38
19	233	234	-2
20	46	45	0
21	91	97	-10

6 2 L

0	164	68	116
1	222	234	-22
2	497	517	-30
3	207	240	-63
4	479	491	-19
5	971	1031	-59
6	516	531	-23
7	643	656	-17
8	139	141	-3
9	488	480	12
10	154	137	23
11	163	155	11
12	420	402	28
13	164	176	-18
14	108	124	-18
15	203	182	34
16	177	164	19
17	208	195	24
18	50	76	-22
19	185	176	19
20	176	178	-4
21	46	48	-2

8 2 L

0	78	75	3
1	382	397	-27
2	572	615	-63
3	414	419	-8
4	101	96	5
5	697	715	-22
6	295	304	-16
7	627	641	-18
8	588	574	19
9	759	754	5
10	83	74	7
11	128	118	11
12	321	289	52
13	82	87	-4
14	113	144	-44
15	300	306	-11
16	279	269	18
17	149	155	-9
18	134	120	24
19	194	194	0
20	86	87	-1

10 2 L

0	463	494	-52
1	141	139	3
2	373	383	-18
3	89	70	19
4	173	176	-4
5	-43	19	-11
6	255	233	33
7	446	420	39
8	78	38	21
9	166	162	5
10	333	309	38
11	108	103	4
12	127	125	2
13	152	143	11
14	317	313	7
15	108	110	-2
16	88	48	36
17	87	91	-5
18	108	107	1
19	54	52	2

12 2 L

0	451	476	-43
1	244	254	-20
2	285	295	-19

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3	920	956	-35	1	140	128	23	10	2**	258	-25
4	692	713	-26	2	261	245	36	11	250	240	17
5	691	704	-16	3	190	178	25	12	163	167	-6
6	212	213	-1	4	80	67	18	13	349	334	26
7	633	621	15	5	402	375	50	14	198	201	-5
8	197	189	12	6	176	159	39	15	345	332	23
9	379	357	35	7	255	2*2	30	16	3*	32	0
10	284	248	58	8	63	23	41	17	150	150	0
11	280	251	46	9	218	199	46	18	110	115	-7
12	39	28	4	10	50	46	5	19	-21	35	-15
13	90	91	-1	11	61	55	9	20	-19	9	-5
14	214	196	33	12	142	145	-9				
15	77	85	-9						5 3 L		
16	39	11	14		20 2 L						
17	261	259	4					1	119	156	-38
18	22	34	-10	0	43	28	14	2	404	401	4
				1	189	181	21	3	319	349	-50
	14 2 L			2	273	253	47	4	108	110	-2
				3	294	285	21	5	193	205	-18
0	384	404	-36	4	74	74	0	6	65	72	-5
1	115	110	7	5	404	380	45	7	76	70	4
2	282	291	-18	6	103	86	38	8	183	172	15
3	135	124	16	7	305	281	56	9	168	154	18
4	66	27	25	8	154	1*9	15	10	3*	74	-21
5	282	275	13	9	273	287	-33	11	205	186	28
6	97	94	3					12	-49	19	-14
7	566	545	30		1 3 L			13	203	200	5
8	127	115	16					14	93	104	-12
9	258	230	53	1	406	428	-40	15	212	208	7
10	236	230	12	2	167	165	3	16	62	52	7
11	215	193	40	3	380	358	40	17	76	88	-13
12	66	52	12	4	18	15	0	18	-18	15	-4
13	45	18	15	5	109	144	40	19	33	33	0
14	214	194	44	6	295	277	35				
15	107	99	15	7	-25	4	-4		7 3 L		
16	25	25	0	8	29	37	-3				
17	80	121	-96	9	416	412	6	1	43	36	2
				10	372	377	-8	2	207	202	7
	16 2 L			11	841	825	16	3	165	147	18
				12	244	226	31	4	55	45	4
0	115	101	21	13	507	505	3	5	73	74	0
1	33	26	3	14	193	197	-7	6	72	36	19
2	105	89	22	15	149	145	6	7	33	47	-5
3	135	1*1	-10	16	17*	180	-10	8	102	114	-11
4	225	218	14	17	50	97	-43	9	-41	14	-8
5	87	82	6	18	-18	16	-4	10	140	156	-20
6	146	139	12	19	26	8	6	11	101	135	-52
7	45	34	6	20	30	7	10	12	127	110	18
8	225	216	19					13	26	5	3
9	95	89	8		3 3 L			14	110	146	-45
10	61	44	16					15	80	91	-11
11	44	37	5	1	1175	1212	-28	16	-27	26	-10
12	125	121	8	2	96	106	-10	17	50	31	12
13	41	22	16	3	676	714	-49	18	27	1	7
14	31	10	1*	*	312	308	7	19	-20	5	-6
15	80	96	-40	5	302	303	-1				
				6	194	201	-12		9 3 L		
	18 2 L			7	100	95	5				
				8	192	196	-6	1	628	652	-31
0	46	48	-1	9	290	264	44	2	160	171	-15

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3	540	563	-33	4	105	92	18	2	162	167	-6
4	135	155	-22	5	167	152	28	3	178	181	-4
5	258	245	18	6	86	78	10	4	301	273	47
6	214	216	-2	7	47	64	-15	5	86	57	19
7	61	55	2	8	101	91	14	6	409	400	13
8	81	71	6	9	208	196	26	7	-9	12	-1
9	409	406	4	10	11	13	0	8	52	61	-5
10	60	100	-28	11	334	307	55	9	194	188	9
11	625	623	2	12	7	1	0	10	197	199	-3
12	48	58	-5	13	251	250	2	11	103	109	-6
13	510	500	14					12	138	123	20
14	22	28	-1		17 3 L			13	-35	37	-15
15	263	250	25					14	129	132	-4
16	142	138	7	1	367	358	18	15	97	103	-8
17	133	154	-44	2	21	27	-2	16	93	111	-27
18	24	46	-21	3	279	267	27	17	43	61	-19
				4	119	113	11				
	11 3 L			5	145	136	19		4 4 L		
				6	99	87	23				
1	787	823	-40	7	-20	27	-12	0	233	243	-12
2	155	160	-7	8	114	96	37	1	79	9	16
3	413	416	-5	9	61	68	-11	2	151	150	0
4	134	157	-30	10	87	80	15	3	150	146	4
5	134	149	-19	11	87	98	-32	4	215	222	-9
6	179	169	14					5	304	308	-6
7	19	20	0		19 3 L			6	230	222	11
8	92	94	-1					7	200	185	20
9	201	177	35	1	91	96	-11	8	87	101	-11
10	147	131	19	2	39	46	-8	9	107	109	-1
11	178	150	38	3	29	9	11	10	136	134	2
12	91	68	20	4	-18	10	-6	11	70	55	10
13	243	211	58	5	26	6	11	12	102	94	9
14	67	88	-24	6	41	52	-17	13	44	23	9
15	175	166	19	7	8	4	1	14	121	115	8
16	33	37	-3					15	-38	18	-13
17	97	102	-11		0 4 L			16	55	56	0
								17	99	99	0
	13 3 L			0	454	494	-60				
				1	56	61	-2		6 4 L		
1	510	522	-18	2	666	602	75				
2	270	286	-31	3	281	246	55	0	443	473	-46
3	156	156	0	4	192	166	37	1	151	160	-10
4	41	19	9	5	720	642	87	2	412	401	15
5	45	30	7	6	460	440	30	3	204	205	-1
6	47	41	3	7	760	713	51	4	151	163	-13
7	38	34	1	8	273	269	6	5	35	53	-6
8	65	42	16	9	261	225	60	6	51	4	12
9	73	68	4	10	280	273	12	7	153	133	21
10	30	16	4	11	161	148	19	8	142	118	26
11	68	77	-9	12	360	361	-1	9	308	305	4
12	20	32	-5	13	127	140	-18	10	281	275	9
13	41	44	-2	14	239	238	1	11	161	164	-4
14	-15	22	-8	15	215	217	-3	12	278	272	10
15	25	45	-20	16	326	326	0	13	6	8	0
				17	253	288	-82	14	171	161	18
	15 3 L							15	41	40	0
					2 4 L			16	114	110	7
1	232	219	25								
2	242	246	-8	0	375	364	12		8 4 L		
3	290	276	28	1	37	45	-2				

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0	300	331	-54	5	40	48	-7	6	267	256	15
1	41	33	3	6	168	173	-10	7	94	60	20
2	315	325	-17	7	87	76	16	8	106	99	5
3	156	144	14	8	93	89	7	9	98	113	-14
4	132	142	-9	9	147	141	15	10	44	11	10
5	365	374	-13	10	121	126	-13	11	89	99	-11
6	88	120	-26	11	77	79	-4	12	117	112	7
7	369	368	1					13	84	77	10
8	149	156	-8		16 4 L						
9	149	133	17						7 5 L		
10	182	158	32	0	23	16	3				
11	99	87	11	1	26	29	-2	1	75	80	-3
12	202	202	0	2	13	11	0	2	86	106	-17
13	88	85	3	3	-27	14	-12	3	-26	58	-16
14	164	156	14	4	56	67	-16	4	73	53	10
15	114	118	-11	5	26	1	10	5	9	24	-1
16	97	134	-127	6	135	129	15	6	153	143	10
				7	54	36	27	7	60	35	9
	10 4 L			8	29	34	-6	8	29	6	3
								9	54	36	8
0	69	79	-8		1 5 L			10	23	23	0
1	59	52	4					11	63	69	-6
2	100	99	1	1	241	230	14	12	49	65	-20
3	-21	39	-11	2	528	468	73				
4	78	76	1	3	249	218	37		9 5 L		
5	44	39	2	4	257	215	55				
6	219	232	-22	5	30	19	2	1	107	123	-19
7	123	137	-17	6	183	164	23	2	285	311	-49
8	52	59	-4	7	37	16	5	3	115	122	-9
9	73	63	7	8	216	205	16	4	307	312	-8
10	33	33	0	9	100	91	9	5	28	15	3
11	43	37	3	10	-41	40	-17	6	312	305	12
12	67	70	-3	11	34	18	5	7	32	40	-3
13	25	16	3	12	-18	38	-11	8	270	268	4
14	31	17	9	13	5	17	-2	9	45	70	-25
				14	-29	13	-10	10	118	115	6
	12 4 L										
					3 5 L				11 5 L		
0	361	372	-20								
1	-22	5	-3	1	67	67	0	1	-6	35	-10
2	299	292	13	2	58	41	5	2	63	57	5
3	255	251	8	3	71	66	2	3	32	47	-9
4	316	323	-13	4	355	352	4	4	199	195	8
5	456	457	-1	5	63	79	-8	5	55	48	6
6	242	238	7	6	422	387	47	6	215	206	20
7	328	322	11	7	-25	28	-5	7	36	6	14
8	131	128	5	8	368	349	29	8	257	260	-7
9	183	173	20	9	76	62	10				
10	223	224	-2	10	301	298	5		13 5 L		
11	105	108	-5	11	16	26	-2				
12	182	186	-10	12	20	2	3	1	27	33	-4
13	43	36	9	13	78	76	2	2	30	23	4
								3	17	3	3
	14 4 L				5 5 L			4	51	66	-22
								5	7	36	-18
0	244	237	15	1	-40	32	-9				
1	84	84	0	2	70	61	3		0 6 L		
2	238	226	27	3	-53	1	-8				
3	48	55	-6	4	161	162	-1	0	252	316	-81
4	20	6	3	5	26	4	2	1	133	147	-13

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2	428	406	28	3	159	183	-23	4	34	44	-3
3	-45	65	-21	4	47	21	7	5	44	56	-5
4	239	269	-46	5	60	56	2				
5	134	166	-45	6	53	67	-10		6 6 L		
6	51	17	14								
					4 6 L			0	143	160	-10
	2 6 L							1	97	97	0
				0	107	111	-1	2	132	131	0
0	-131	79	-15	1	-31	42	-4	3	117	155	-49
1	113	160	-10	2	-6	51	-5				
2	-69	32	-16	3	-21	57	-11				

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0 0 L

4	3224	3230	-1
6	1829	1810	9
8	1514	1484	17
10	2857	2862	-1
12	653	643	7
14	2277	2287	-4
16	639	659	-12
18	1170	1180	-6
20	833	822	6
22	333	327	2
24	1068	1061	3
26	271	276	-1
28	510	493	7
30	171	103	10
32	-141	113	-16
34	127	75	5
36	-53	39	-2

2 0 L

2	2383	2327	31
4	3848	3847	0
6	2691	2675	8
8	2064	2036	18
10	2560	2542	9
12	702	729	-28
14	1698	1695	2
16	744	743	0
18	986	977	8
20	762	765	-2
22	906	921	-12
24	412	380	18
26	118	83	5
28	300	299	0
30	130	173	-9
32	170	172	0
34	250	224	8
36	-70	60	-5

4 0 L

0	2350	2340	5
2	3485	3526	-16
4	2228	2222	3
6	2321	2296	14
8	2024	2021	1
10	915	925	-11
12	2507	2484	12
14	1041	1045	-3
16	1224	1234	-8
18	751	745	5
20	613	626	-11
22	581	562	14
24	360	359	0
26	501	472	18
28	221	241	-6
30	300	254	19
32	210	198	3
34	-36	34	-1
36	26	103	-6

6 0 L

0	1799	1769	21
2	3603	3731	-50
4	1175	1174	1
6	2220	2212	4
8	2472	2476	-2
10	1343	1313	25
12	1809	1835	-17
14	433	398	26
16	1566	1570	-2
18	754	750	3
20	657	658	0
22	560	552	6
24	268	282	-5
26	617	609	5
28	188	104	19
30	250	211	13
32	-97	62	-9
34	213	195	5
36	-100	119	-16

8 0 L

0	155	117	19
2	3425	3466	-16
4	1662	1651	8
6	2136	2149	-8
8	2071	2087	-10
10	828	827	1
12	2073	2062	6
14	568	585	-14
16	1275	1281	-5
18	579	597	-15
20	554	552	1
22	966	971	-4
24	120	66	8
26	412	395	9
28	168	122	10
30	300	273	11
32	193	195	0
34	78	80	0

10 0 L

0	2933	2933	0
2	1569	1587	-10
4	1865	1880	-7
6	1596	1600	-2
8	1344	1345	0
10	1233	1259	-15
12	1454	1452	1
14	1222	1212	5
16	751	769	-11
18	717	716	0
20	629	628	0
22	261	219	11
24	505	548	-19
26	333	328	1
28	312	296	4
30	225	182	9
32	203	148	10
34	-29	10	0

12 0 L

0	2562	2630	-25
2	656	599	40
4	2197	2211	-5
6	1439	1446	-3
8	1152	1133	11
10	2432	2476	-16
12	374	394	-9
14	1489	1519	-16
16	436	461	-13
18	868	891	-14
20	659	678	-10
22	294	324	-9
24	588	544	21
26	154	65	11
28	267	311	-12
30	139	92	5
32	-177	50	-17
34	356	335	6

14 0 L

0	2380	2389	-3
2	701	698	8
4	1886	1891	-2
6	1184	1180	2
8	822	828	-3
10	1027	1023	2
12	1024	1046	-13
14	1368	1388	-11
16	344	343	0
18	626	644	-10
20	493	474	8
22	202	231	-6
24	529	537	-3
26	-85	134	-13
28	364	328	11
30	128	148	-2
32	220	234	-2

16 0 L

0	1004	946	34
2	1269	1307	-22
4	1164	1165	0
6	1099	1109	-6
8	1061	1108	-29
10	1133	1135	-1
12	585	588	-1
14	646	664	-10
16	606	607	0

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18	584	592	-4	22	263	284	-5	10	244	186	12
20	408	443	-14	24	153	147	0	12	270	294	-6
22	512	522	-4	26	218	198	4	14	-92	126	-11
24	169	212	-8	28	168	143	3	16	287	264	6
26	243	234	2					18	230	165	13
28	222	192	6		24 0 L			20	-96	113	-10
30	-87	135	-12								
32	-148	71	-13	0	1392	1355	18		32 0 L		
				2	33	37	0				
	18 0 L			4	729	742	-7	0	234	179	11
				6	491	488	1	2	589	550	17
0	615	682	-42	8	326	356	-10	4	107	79	2
2	1522	1507	7	10	686	673	6	6	304	247	15
4	540	537	1	12	203	204	0	8	248	313	-16
6	945	955	-6	14	637	641	-1	10	-122	54	-9
8	1093	1119	-15	16	184	206	-4	12	531	471	24
10	470	453	8	18	313	342	-9	14	-184	15	-16
12	1059	1081	-13	20	330	333	0	16	270	269	0
14	286	253	10	22	158	35	12				
16	858	863	-2	24	408	413	-1		34 0 L		
18	425	421	1	26	-145	99	-15				
20	373	368	1					0	144	200	-9
22	276	279	0		26 0 L			2	277	214	14
24	177	213	-7					4	76	107	-2
26	376	371	1	0	507	514	-2	6	218	192	5
28	-84	110	-9	2	164	227	-13	8	135	189	-8
30	-98	166	-17	4	757	731	13	10	-118	134	-15
				6	417	400	6	12	266	202	14
	20 0 L			8	233	261	-7				
				10	676	638	18		36 0 L		
0	-88	106	-12	12	26	38	0				
2	1582	1552	15	14	619	591	13	0	210	168	7
4	487	489	-1	16	-177	92	-20	2	182	97	12
6	895	890	3	18	339	313	8	4	185	179	1
8	937	923	8	20	125	184	-9				
10	-52	22	-2	22	315	326	-3		1 1 L		
12	1345	1364	-9	24	145	144	0				
14	128	120	1					1	350	315	51
16	710	692	9		28 0 L			2	366	315	69
18	220	251	-7					3	1549	1534	12
20	204	274	-17	0	771	758	6	4	2239	2228	6
22	541	543	0	2	137	135	0	5	1209	1181	28
24	99	70	2	4	450	427	9	6	956	945	12
26	336	309	7	6	360	299	20	7	127	142	-8
28	187	67	15	8	261	309	-13	8	197	200	-2
30	212	179	6	10	393	369	8	9	264	269	-4
				12	260	228	7	10	490	483	7
	22 0 L			14	302	335	-9	11	202	182	10
				16	207	179	5	12	81	5	8
0	502	527	-12	18	242	263	-5	13	287	284	1
2	813	811	1	20	251	233	4	14	-94	24	-9
4	621	607	7	22	83	19	3	15	230	214	7
6	674	663	6					16	-9	158	-18
8	617	613	2		30 0 L			18	596	628	-31
10	701	712	-5					20	285	319	-12
12	375	352	8	0	136	67	7				
14	384	390	-2	2	508	470	15		3 1 L		
16	519	482	16	4	83	180	-12				
18	323	346	-7	6	334	296	12	1	1137	1161	-25
20	289	348	-17	8	340	333	2	2	802	817	-18

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3	+36	477	-55	15	129	132	0	+	120	0	11
4	396	453	-78	16	80	87	-1	5	191	103	19
5	197	140	42	17	80	143	-14	6	531	536	-3
6	1473	1473	0	18	113	34	12	7	561	539	13
7	492	460	40	19	125	150	-6	8	434	467	-18
8	1418	1387	27	20	99	30	9	9	115	190	-16
9	520	510	11	21	-57	15	-3	10	74	3	4
10	490	490	0					11	-190	14	-28
11	512	521	-9		9 1 L			12	-22	9	0
12	273	257	9					13	-93	93	-13
13	520	518	1	1	692	706	-17	14	188	196	-2
14	238	253	-7	2	505	513	-9	15	436	427	4
15	554	543	9	3	854	833	23	16	460	456	2
16	558	578	-17	4	1348	1345	2	17	117	99	2
17	345	344	0	5	510	499	11	18	132	1	11
18	239	232	3	6	969	979	-7	19	-146	0	-13
19	78	144	-14	7	-54	3	-2	20	-75	17	-3
20	325	331	-3	8	686	678	5	21	150	60	11
21	73	134	-11	9	360	368	-3				
				10	539	541	-1		15 1 L		
	5 1 L			11	402	405	-1				
				12	164	154	2	1	507	524	-9
1	736	759	-30	13	513	513	0	2	340	350	-4
2	364	379	-19	14	33	150	-16	3	318	325	-3
3	58	123	-26	15	202	224	-7	4	636	673	-23
4	563	576	-18	16	296	269	11	5	339	320	8
5	139	154	-9	17	102	53	5	6	416	442	-14
6	213	272	-54	18	588	592	-2	7	126	203	-18
7	421	400	24	19	170	179	-2	8	307	299	3
8	261	279	-15	20	348	399	-20	9	109	88	3
9	-54	33	-6	21	-37	49	-2	10	472	442	16
10	474	470	3					11	481	478	1
11	538	518	18		11 1 L			12	41	37	0
12	-88	57	-12					13	161	173	-2
13	181	204	-9	1	544	540	2	14	-44	37	-2
14	73	39	4	2	386	394	-4	15	-94	59	-8
15	-33	1	-1	3	362	373	-6	16	-148	+2	-15
16	-147	23	-25	4	365	377	-6	17	134	59	9
17	-24	28	-1	5	35	89	-5	18	350	333	6
18	218	218	0	6	941	953	-8	19	78	+3	2
19	132	139	-1	7	378	385	-3	20	349	314	12
20	239	245	-2	8	982	988	-3				
21	-15	91	-8	9	490	465	14		17 1 L		
				10	338	286	22				
	7 1 L			11	168	203	-9	1	459	436	13
				12	125	193	-16	2	273	263	4
1	314	317	-3	13	470	454	9	3	159	174	-3
2	87	115	-11	14	225	265	-13	4	277	308	-12
3	248	237	10	15	464	457	3	5	112	32	8
4	238	205	27	16	504	502	1	6	546	548	-1
5	281	249	29	17	341	352	-4	7	189	149	9
6	97	84	4	18	253	227	8	8	504	519	-8
7	318	296	18	19	-90	13	-5	9	148	142	1
8	173	161	5	20	239	171	17	10	345	310	14
9	115	34	16					11	377	346	13
10	109	122	-3		13 1 L			12	-67	115	-12
11	154	210	-22					13	216	245	-8
12	82	57	3	1	132	54	11	14	161	85	12
13	117	98	4	2	-24	109	-9	15	319	287	11
14	-98	5	-10	3	74	100	-3	16	182	246	-15

17	196	116	14	4	229	129	21	9	490	483	6
18	95	100	0	5	92	161	-9	10	328	309	12
19	165	148	2					11	71	14	5
					0 2 L			12	506	468	30
	19 1 L							13	156	121	10
				0	1311	1357	-32	14	231	268	-18
1	76	28	3	1	251	244	5	15	161	196	-13
2	104	44	6	2	250	264	-10	16	379	343	25
3	46	184	-23	3	1254	1277	-16	17	173	111	18
4	163	179	-3	4	980	987	-5	18	211	225	-5
5	14	143	-13	5	868	871	-2	19	383	412	-18
6	241	235	1	6	426	425	1	20	93	40	6
7	66	174	-16	7	1917	1898	12				
8	182	119	13	8	649	607	47		6 2 L		
9	-149	49	-16	9	1395	1369	15				
10	-130	73	-14	10	854	810	31	0	141	30	35
11	-174	12	-20	11	585	593	-5	1	314	296	17
12	148	7	14	12	170	126	9	2	596	616	-25
13	93	11	5	13	621	609	7	3	192	201	-6
14	89	6	4	14	1146	1138	4	4	600	582	21
15	224	211	3	15	529	565	-20	5	1228	1231	-2
16	218	157	12	16	-178	118	-32	6	624	629	-5
17	-188	46	-19	17	568	578	-6	7	728	725	3
				19	295	339	-17	8	298	226	45
	21 1 L							9	638	633	4
					2 2 L			10	193	180	5
1	226	284	-18					11	210	185	10
2	159	215	-14	0	602	634	-46	12	619	567	46
3	311	306	1	1	55	21	6	13	225	276	-25
4	411	428	-8	2	116	1	32	14	140	162	-7
5	68	41	1	3	931	930	1	15	356	342	9
6	538	567	-15	4	774	769	6	16	325	286	22
7	195	187	1	5	597	591	7	17	336	331	3
8	532	508	11	6	468	471	-3	18	-71	69	-9
9	316	278	12	7	461	472	-12	19	362	370	-4
10	213	211	0	8	1038	1024	14	20	319	305	7
11	186	113	13	9	251	201	28	21	119	120	0
12	88	68	1	10	399	377	17				
13	288	305	-5	11	344	367	-16		8 2 L		
14	159	176	-3	12	174	100	22				
				13	164	121	13	0	116	64	14
	23 1 L			14	98	0	10	1	504	485	20
				15	213	188	11	2	735	749	-15
1	313	315	0	16	202	212	-4	3	457	448	9
2	224	248	-6	17	408	390	12	4	189	142	21
3	366	337	11	18	338	316	12	5	897	901	-4
4	524	479	20	19	223	255	-13	6	407	394	10
5	133	210	-14	20	298	299	0	7	725	729	-3
6	382	394	-4					8	786	768	17
7	213	91	22		4 2 L			9	1008	996	10
8	272	296	-7					10	170	82	22
9	181	177	0	0	517	527	-13	11	81	114	-6
10	192	234	-9	1	637	624	17	12	475	455	15
11	229	187	10	2	1095	1094	1	13	-69	87	-13
				3	589	551	49	14	110	172	-18
	25 1 L			4	153	4	46	15	458	467	-6
				5	796	775	25	16	441	423	12
1	116	64	5	6	371	374	-3	17	207	224	-6
2	-75	30	-3	7	140	112	11	18	207	211	-1
3	-160	97	-20	8	367	363	3	19	404	405	0

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20	249	149	35	5	344	391	-22		20	2	L	
21	229	221	2	6	136	143	-1					
				7	837	836	0	0	-62	34		-3
	10	2	L	8	179	160	4	1	380	355		11
				9	320	321	0	2	476	486		-4
0	570	602	-22	10	400	391	4	3	446	460		-6
1	308	251	26	11	343	347	-1	4	119	118		0
2	568	539	20	12	211	82	27	5	684	666		10
3	177	92	20	13	-94	69	-9	6	237	165		18
4	222	228	-2	14	398	389	3	7	500	472		13
5	190	100	20	15	119	176	-11	8	328	326		0
6	293	312	-8	16	-137	70	-15	9	609	581		14
7	560	507	32	17	276	308	-10	10	-123	15		-8
8	149	74	12	18	351	343	2	11	241	134		24
9	202	139	15	19	90	0	4	12	343	297		15
10	456	418	20	20	10	148	-12	13	90	46		3
11	203	169	9					14	169	99		10
12	285	226	23		16	2	L					
13	257	238	6						22	2	L	
14	465	467	-1	0	241	190	16					
15	63	99	-4	1	-79	58	-7	0	154	151		0
16	117	129	-1	2	113	123	-1	1	67	34		2
17	127	150	-4	3	213	281	-24	2	-81	48		-5
18	178	194	-3	4	405	370	17	3	216	168		11
19	204	115	19	5	-101	121	-17	4	307	247		19
20	106	43	5	6	284	257	9	5	-92	119		-12
21	219	32	29	7	168	11	20	6	152	148		0
				8	393	357	16	7	98	46		4
	12	2	L	9	171	159	2	8	185	151		6
				10	50	125	-8	9	170	154		2
0	606	620	-8	11	58	87	-2	10	96	96		0
1	306	290	6	12	161	194	-7	11	94	6		5
2	382	352	14	13	194	2	25					
3	1176	1230	-33	14	84	43	3		24	2	L	
4	929	933	-2	15	240	181	14					
5	822	813	5	16	206	163	9	0	305	264		12
6	388	350	18	17	-86	44	-5	1	-113	3		-7
7	852	857	-3	18	-145	59	-13	2	154	34		13
8	285	275	3					3	239	266		-7
9	448	458	-5		18	2	L	4	280	174		26
10	431	416	7					5	251	246		1
11	425	399	13	0	61	15	2					
12	-112	46	-10	1	161	206	-10		1	3	L	
13	144	154	-2	2	430	394	18					
14	309	322	-5	3	193	208	-4	1	524	505		21
15	104	115	-1	4	192	162	7	2	197	160		19
16	-6	11	0	5	595	609	-8	3	398	385		12
17	502	492	5	6	274	264	3	4	130	13		23
18	187	84	17	7	347	327	8	5	252	207		26
19	508	538	-14	8	-37	63	-3	6	361	322		30
20	424	398	10	9	351	329	9	7	143	40		22
21	494	469	11	10	-150	92	-19	8	157	69		22
				11	94	66	2	9	535	526		7
	14	2	L	12	275	296	-6	10	486	457		23
				13	210	152	12	11	986	1003		-15
0	624	627	-1	14	224	129	20	12	327	354		-17
1	169	200	-8	15	224	154	15	13	697	697		0
2	412	412	0	16	121	172	-7	14	263	275		-6
3	151	217	-16	17	255	193	15	15	218	247		-12
4	102	78	3					16	241	263		-10

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17	99	125	-5	8	185	165	7		13	3	L	
18	94	7	9	9	68	18	4					
19	-98	23	-9	10	165	209	-17	1	584	648	-41	
20	53	23	2	11	173	154	6	2	425	441	-8	
				12	186	168	6	3	216	192	7	
	3	3	L	13	-155	13	-25	4	145	41	14	
				14	234	203	13	5	-127	21	-12	
1	1416	1390	21	15	117	128	-2	6	112	54	7	
2	220	151	36	16	41	46	0	7	108	55	6	
3	872	865	7	17	-92	81	-14	8	177	75	18	
4	369	350	15	18	-104	13	-9	9	-156	50	-18	
5	372	343	23	19	-65	0	-3	10	146	52	13	
6	258	225	18	20	-95	134	-22	11	112	95	2	
7	166	125	13					12	-175	34	-21	
8	255	236	10		9	3	L	13	79	49	2	
9	413	362	36					14	133	15	11	
10	367	342	17	1	801	812	-7	15	163	69	13	
11	428	414	10	2	189	203	-3	16	205	13	25	
12	135	198	-22	3	692	685	4	17	105	0	6	
13	524	522	1	4	161	152	2	18	138	57	8	
14	209	243	-15	5	348	319	12	19	145	22	11	
15	530	530	0	6	276	258	6					
16	-76	39	-7	7	198	94	23		15	3	L	
17	260	279	-6	8	108	94	2					
18	186	193	-2	9	552	579	-17	1	377	325	23	
19	32	50	-1	10	124	120	0	2	399	391	4	
20	-118	21	-12	11	845	867	-14	3	426	402	11	
				12	80	130	-7	4	158	109	9	
	5	3	L	13	745	775	-19	5	166	237	-18	
				14	-42	63	-4	6	99	114	-2	
1	222	232	-5	15	414	425	-5	7	122	97	3	
2	500	485	14	16	232	211	5	8	210	158	13	
3	449	419	26	17	209	258	-14	9	339	331	3	
4	117	114	0	18	110	72	4	10	113	22	8	
5	284	251	19	19	-144	9	-12	11	513	536	-11	
6	79	75	0	20	94	67	2	12	216	19	30	
7	134	85	11					13	521	454	34	
8	257	231	12		11	3	L	14	132	53	8	
9	308	233	41					15	386	364	8	
10	134	99	8	1	1077	1105	-17	16	169	88	12	
11	307	302	3	2	254	249	1	17	119	134	-2	
12	63	37	2	3	603	609	-3					
13	331	323	5	4	145	205	-15		17	3	L	
14	203	141	22	5	182	194	-3					
15	326	343	-10	6	240	204	11	1	561	589	-15	
16	0	65	-4	7	-178	50	-24	2	-161	22	-17	
17	185	159	8	8	-43	113	-10	3	430	434	-1	
18	59	34	2	9	292	285	2	4	211	168	11	
19	142	56	15	10	204	207	0	5	214	220	-1	
20	234	190	15	11	334	298	14	6	-76	114	-12	
				12	105	94	1	7	-127	73	-13	
	7	3	L	13	406	409	-1	8	168	159	1	
				14	-125	117	-19	9	-16	153	-14	
1	128	24	18	15	310	321	-4	10	173	159	2	
2	277	254	13	16	120	46	7	11	269	227	12	
3	228	164	27	17	257	220	10	12	145	74	9	
4	44	69	-3	18	34	142	-11	13	332	242	29	
5	157	71	21	19	169	8	17	14	84	133	-6	
6	148	37	22	20	127	47	7	15	328	302	8	
7	174	26	31					16	-242	54	-32	

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19 3 L

1	179	225	-11
2	48	106	-5
3	-42	62	-3
4	-144	11	-12
5	148	27	13
6	-68	98	-8
7	-145	6	-12
8	-101	40	-6
9	115	75	4
10	208	74	22
11	225	206	4
12	-126	103	-15
13	66	108	-4

21 3 L

1	647	625	11
2	131	103	3
3	386	375	4
4	41	63	-1
5	162	119	6
6	190	123	11
7	-90	54	-6
8	-77	5	-3
9	286	268	5
10	-54	5	-1

23 3 L

1	327	319	2
2	157	145	2
3	272	296	-6

0 4 L

0	628	633	-3
1	131	70	10
2	724	738	-10
3	353	345	4
4	232	215	5
5	929	934	-3
6	520	517	1
7	871	899	-19
8	248	284	-14
9	377	354	12
10	412	408	2
11	230	202	9
12	566	543	14
13	168	168	0
14	318	362	-19
15	339	374	-15
16	488	571	-45
17	515	515	0
18	306	321	-5
19	282	253	8
20	-119	196	-28

2 4 L

0	484	478	5
1	169	125	15
2	236	221	8
3	225	211	6
4	376	370	4
5	121	109	3
6	458	493	-30
7	-127	40	-21
8	-40	116	-18
9	293	285	5
10	268	282	-8
11	135	131	1
12	190	197	-2
13	-54	33	-4
14	256	263	-3
15	44	93	-7
16	158	163	-1
17	105	69	6
18	236	190	17
19	145	137	1
20	135	47	14

4 4 L

0	278	312	-21
1	-5	29	-1
2	203	186	7
3	201	208	-3
4	175	267	-44
5	369	384	-11
6	286	311	-15
7	264	292	-17
8	112	135	-6
9	146	118	8
10	204	183	9
11	112	92	4
12	175	152	8
13	-80	23	-7
14	180	188	-3
15	-51	53	-5
16	-32	61	-4
17	222	191	11
18	173	124	13
19	190	133	15
20	-37	6	-1

6 4 L

0	569	608	-38
1	204	208	-1
2	564	563	0
3	333	320	8
4	197	248	-25
5	93	83	2
6	-143	11	-23
7	277	249	16
8	175	194	-7
9	434	438	-3
10	376	392	-11
11	258	249	4
12	453	442	8
13	84	48	5
14	309	314	-2
15	-114	39	-14
16	204	203	0
17	126	57	11
18	-83	57	-8
19	180	154	7
20	-75	59	-7

8 4 L

0	402	441	-31
1	-73	20	-7
2	437	436	0
3	247	264	-9
4	189	183	2
5	525	554	-26
6	133	134	0
7	553	557	-3
8	204	195	3
9	172	210	-15
10	245	249	-1
11	133	153	-5
12	308	338	-18
13	-85	83	-14
14	260	254	2
15	217	210	2
16	303	279	12
17	314	334	-10
18	177	144	8
19	185	146	10

10 4 L

0	89	79	1
1	-74	66	-8
2	163	125	9
3	-158	23	-19
4	51	101	-5
5	-23	57	-2
6	296	337	-17
7	108	129	-3
8	68	46	1
9	-106	97	-14
10	136	41	12
11	-98	33	-7
12	-61	106	-10
13	-42	15	-1
14	-163	22	-17
15	-238	100	-39
16	135	194	-10
17	108	37	6
18	90	176	-12

12 4 L

0	552	571	-11

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1	57	42	1
2	396	397	0
3	360	369	-9
4	483	475	4
5	718	726	-5
6	382	398	-7
7	551	526	14
8	169	195	-6
9	297	290	2
10	377	372	2
11	222	158	17
12	346	316	12
13	-132	65	-13
14	303	341	-13
15	144	154	-1
16	-162	26	-15
17	401	386	21

14 4 L

0	325	374	-21
1	111	164	-10
2	367	399	-15
3	72	126	-7
4	60	47	0
5	65	8	3
6	255	310	-19
7	86	152	-10
8	178	145	7
9	244	299	-18
10	255	237	5
11	189	141	10
12	298	307	-3
13	186	0	21
14	252	212	10
15	-91	4	-4

16 4 L

0	-163	49	-19
1	-45	29	-2
2	64	36	1
3	-193	16	-24
4	79	110	-3
5	26	40	0
6	294	229	22
7	-59	37	-3
8	206	41	26
9	-199	32	-24
10	-95	0	-5
11	66	4	2
12	-91	16	-5
13	-122	32	-9

18 4 L

0	338	349	-4
1	163	96	10
2	316	263	18
3	162	174	-2
4	206	171	7
5	124	93	4
6	145	93	7
7	129	157	-4
8	90	107	-1
9	239	228	2
10	274	199	20
11	42	133	-9

20 4 L

0	343	338	1
1	68	15	2
2	329	312	5
3	260	233	7
4	182	221	-8
5	491	463	12
6	82	76	0

1 5 L

1	407	368	27
2	645	647	-1
3	287	247	20
4	330	289	24
5	39	15	1
6	257	259	0
7	-51	26	-3
8	328	335	-4
9	183	65	28
10	-111	76	-16
11	-73	50	-7
12	78	92	-2
13	68	18	3
14	-113	32	-11
15	99	4	8
16	182	150	8
17	50	82	-3
18	186	118	16

3 5 L

1	167	74	23
2	168	93	20
3	165	47	26
4	577	567	8
5	107	93	2
6	632	616	13
7	-20	17	0
8	593	575	15
9	155	102	13
10	492	507	-10
11	151	89	13
12	-139	2	-17
13	197	135	18
14	231	217	5
15	130	101	5
16	241	217	8
17	-108	37	-10

5 5 L

1	115	41	11
2	46	116	-11
3	165	19	26
4	296	277	10
5	-37	12	-1
6	454	438	11
7	-115	55	-15
8	214	198	6
9	161	159	0
10	41	7	1
11	200	162	12
12	222	180	15
13	179	91	20
14	79	77	0
15	-32	7	0
16	187	187	0
17	86	50	3

7 5 L

1	141	149	-2
2	189	143	15
3	72	63	1
4	157	98	14
5	100	23	9
6	224	230	-2
7	-43	27	-2
8	145	22	19
9	-47	80	-7
10	60	27	2
11	94	130	-7
12	-47	39	-8
13	43	42	0
14	123	41	11
15	-96	22	-7
16	112	99	2

9 5 L

1	263	222	13
2	481	486	-2
3	134	166	-6
4	465	491	-12
5	-126	25	-10
6	532	518	7
7	110	98	6
8	490	474	7
9	-68	57	-4
10	230	214	4
11	-131	29	-10
12	169	104	10
13	88	12	4
14	87	52	2
15	69	31	2

11 5 L

1	148	17	14

2	91	108	-2
3	135	34	10
4	405	385	8
5	203	69	23
6	377	385	-3
7	-84	18	-4
8	463	483	-9
9	241	176	15
10	481	473	3
11	217	163	11
12	117	52	6
13	180	163	2
14	303	252	14

13 5 L

1	157	54	13
2	-43	8	-1
3	125	14	9
4	58	101	-3
5	179	47	17
6	-204	20	-23
7	-59	53	-3
8	261	229	8
9	178	251	-16
10	298	312	-4
11	242	269	-7
12	170	170	0

15 5 L

1	37	75	-2
2	273	260	3
3	-79	105	-9
4	347	335	4
5	71	28	2
6	411	435	-9
7	64	47	1
8	210	224	-3
9	-64	160	-15
10	135	22	9

17 5 L

1	117	67	5
2	-106	55	-8
3	-119	38	-8
4	283	283	0
5	167	25	14
6	318	338	-5

0 6 L

0	512	510	1
1	189	197	-2
2	702	706	-2
3	129	106	3
4	488	489	0
5	265	233	10
6	-27	57	-2
7	296	231	22
8	144	101	6
9	203	159	10
10	186	223	-9
11	123	46	8
12	372	340	12
13	102	74	3

2 6 L

0	228	216	5
1	204	225	-9
2	130	13	18
3	344	302	24
4	49	22	1
5	87	133	-9
6	-138	125	-31
7	-55	97	-11
8	-12	124	-13
9	147	15	20
10	197	181	5
11	81	10	5
12	108	150	-9
13	63	30	2

4 6 L

0	208	203	2
1	-95	53	-11
2	157	104	14
3	71	91	-3
4	-115	90	-19
5	119	100	3
6	-60	49	-5
7	-118	40	-14
8	169	184	-4
9	123	87	6
10	215	171	14
11	75	7	4
12	102	160	-12

6 6 L

0	358	353	2
1	178	160	5
2	311	270	20
3	166	271	-39
4	106	122	-3
5	191	193	0
6	151	89	13
7	250	228	9
8	-88	26	-7
9	292	261	13
10	-66	173	-27
11	101	41	7

8 6 L

0	301	327	-12
1	-94	86	-14
2	388	392	-2
3	92	25	6
4	264	283	-8
5	99	153	-11
6	-74	11	-4
7	34	128	-12
8	135	118	3
9	-117	64	-15
10	176	147	7

10 6 L

0	174	92	13
1	74	76	0
2	178	179	0
3	113	64	5
4	-88	104	-10
5	130	7	10
6	-144	38	-13
7	-21	43	-1
8	0	63	-2

12 6 L

0	408	376	12
1	-175	71	-20
2	282	261	6
3	214	145	15
4	219	209	2
5	122	133	-10

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0 0 L

4	3297	3282	6
6	1935	1915	13
8	1625	1589	28
10	3129	3135	-2
12	779	752	29
14	2682	2685	-1
16	870	880	-8
18	1546	1559	-9
20	1225	1237	-9
22	179	199	-6
24	1609	1609	0
26	436	481	-24
28	927	926	0
30	333	325	3
32	377	357	8
34	358	357	0
36	168	185	-3

2 0 L

2	2385	2329	31
4	3931	3904	8
6	2805	2768	19
8	2189	2151	23
10	2821	2795	11
12	881	901	-20
14	2050	2050	0
16	1001	998	2
18	1305	1331	-21
20	1136	1119	14
22	1257	1274	-12
24	766	768	-1
26	310	303	3
28	663	666	-1
30	444	433	5
32	446	433	6
34	518	503	7
36	240	233	2

4 0 L

0	2399	2390	5
2	3522	3551	-10
4	2308	2306	1
6	2435	2407	16
8	2182	2179	1
10	1067	1090	-23
12	2836	2785	22
14	1308	1305	2
16	1570	1578	-5
18	1049	1051	-1
20	951	952	0
22	944	944	0
24	636	650	-10
26	844	852	-6
28	487	503	-9
30	588	558	18
32	510	490	10
34	170	135	7
36	394	339	23

6 0 L

0	1889	1856	22
2	3726	3827	-40
4	1270	1260	9
6	2348	2344	2
8	2676	2684	-3
10	1511	1474	29
12	2135	2169	-20
14	567	553	12
16	1987	1986	0
18	1057	1067	-8
20	961	975	-12
22	935	943	-6
24	489	491	-1
26	1083	1083	0
28	256	304	-18
30	555	541	8
32	295	279	5
34	477	436	21

8 0 L

0	146	106	16
2	3587	3630	-16
4	1773	1761	8
6	2308	2306	1
8	2324	2343	-10
10	993	985	7
12	2456	2444	6
14	791	770	19
16	1650	1664	-9
18	876	893	-14
20	843	845	-1
22	1455	1458	-2
24	197	244	-15
26	813	802	8
28	317	334	-7
30	598	584	8
32	481	464	9
34	246	263	-5

10 0 L

0	3082	3090	-3
2	1774	1786	-8
4	2018	2034	-10
6	1780	1795	-10
8	1550	1558	-6
10	1439	1446	-5
12	1766	1776	-6
14	1521	1537	-11
16	1068	1090	-19
18	1023	1041	-15
20	930	943	-10
22	518	497	13
24	898	910	-9
26	602	626	-15
28	589	594	-3
30	473	453	10
32	472	422	26
34	242	169	20

12 0 L

0	2757	2823	-34
2	791	755	37
4	2420	2446	-14
6	1678	1680	-1
8	1389	1381	4
10	2827	2890	-20
12	305	297	2
14	1882	1898	-7
16	673	689	-8
18	1249	1267	-9
20	1093	1062	17
22	560	561	0
24	1010	968	20
26	189	233	-8
28	726	681	20
30	314	296	4
32	-64	226	-19
34	780	688	39

14 0 L

0	2704	2748	-22
2	873	853	12
4	2158	2178	-8
6	1415	1413	1
8	1002	1003	0
10	1338	1352	-7
12	1277	1309	-17
14	1830	1861	-13
16	528	554	-12
18	958	975	-9
20	798	812	-6
22	424	435	-4
24	956	956	0
26	232	313	-16
28	705	695	4
30	333	365	-7
32	512	517	-1

16 0 L

0	1258	1215	33
2	1476	1514	-20
4	1465	1477	-6
6	1408	1417	-4
8	1372	1387	-8
10	1477	1487	-5
12	788	793	-2
14	967	987	-11
16	903	913	-5
18	901	908	-3

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20	755	755	0	24	241	355	-24	12	579	556	9
22	843	851	-3	26	501	468	12	14	370	326	12
24	504	511	-2	28	305	336	-7	16	454	535	-25
26	494	480	5					18	412	409	0
28	438	442	-1		24 0 L			20	389	332	16
30	388	377	3								
32	359	283	18	0	1862	1850	7		32 0 L		
				2	240	290	-11				
	18 0 L			4	1033	1036	-1	0	93	96	0
				6	759	762	-1	2	995	941	24
0	934	979	-39	8	622	619	1	4	363	305	16
2	1844	1837	3	10	1024	1010	7	6	545	520	9
4	782	766	9	12	486	482	1	8	633	609	9
6	1226	1227	0	14	1032	1012	9	10	227	65	21
8	1449	1456	-3	16	445	437	2	12	932	862	31
10	703	725	-11	18	650	656	-2	14	187	132	7
12	1437	1458	-10	20	627	622	2	16	594	567	9
14	450	465	-6	22	137	68	6				
16	1241	1245	-2	24	791	763	12		34 0 L		
18	718	710	3	26	266	297	-6				
20	643	661	-8					0	434	443	-3
22	637	574	31		26 0 L			2	512	516	-1
24	388	417	-8					4	334	279	13
26	767	751	7	0	773	791	-11	6	461	441	6
28	309	308	0	2	448	434	4	8	466	464	0
30	453	415	12	4	1163	1155	3	10	336	309	7
				6	736	719	7	12	552	511	14
	20 0 L			8	496	511	-5				
				10	1060	1043	8		36 0 L		
0	75	41	3	12	147	165	-2				
2	1950	1968	-7	14	1018	983	17	0	381	354	10
4	699	744	-24	16	278	268	2	2	344	328	4
6	1204	1209	-2	18	556	592	-13	4	473	424	15
8	1247	1260	-7	20	408	456	-14				
10	161	156	0	22	589	618	-10		1 1 L		
12	1883	1889	-2	24	391	415	-6				
14	248	300	-12					1	344	315	37
16	1062	1075	-6		28 0 L			2	367	305	76
18	476	504	-10					3	1541	1521	16
20	542	508	14	0	1264	1252	7	4	2291	2250	24
22	926	948	-10	2	354	338	4	5	1241	1204	35
24	172	210	-5	4	749	738	5	6	986	970	18
26	620	658	-13	6	544	570	-10	7	164	149	8
28	293	224	15	8	519	546	-9	8	249	228	17
30	465	457	2	10	724	700	10	9	293	289	3
				12	463	449	4	10	518	493	28
	22 0 L			14	723	691	14	11	210	195	7
				16	407	402	1	12	32	2	1
0	666	703	-27	18	553	530	8	13	339	322	7
2	1182	1187	-2	20	494	494	0	14	98	42	5
4	911	889	12	22	76	135	-5	15	190	244	-18
6	994	982	6					16	214	221	-3
8	1006	984	11		30 0 L			17	190	192	0
10	1002	997	2					18	746	757	-10
12	627	644	-7	0	288	305	-5	19	310	355	-27
14	570	617	-19	2	776	774	0	20	375	394	-13
16	853	826	13	4	418	438	-6	21	-10	68	-5
18	587	616	-11	6	632	580	22	22	85	73	2
20	604	620	-6	8	670	632	15	23	-65	24	-4
22	637	616	8	10	478	465	4	24	199	137	21

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25	313	324	-5	25	117	101	3
26	272	278	-2	26	-81	0	-6
27	281	327	-21	27	118	73	8

3 1 L

1	1134	1160	-27
2	813	835	-27
3	456	503	-59
4	429	488	-75
5	204	153	33
6	1538	1526	9
7	510	464	54
8	1490	1450	32
9	545	538	7
10	514	519	-4
11	567	564	3
12	239	268	-17
13	606	596	8
14	356	309	26
15	621	619	1
16	667	681	-13
17	391	409	-13
18	330	345	-9
19	153	154	0
20	430	455	-20
21	181	172	3
22	402	424	-15
23	240	247	-3
24	148	117	7
25	171	174	0
26	177	116	17
27	49	48	0

5 1 L

1	755	786	-39
2	402	407	-6
3	125	136	-5
4	611	616	-6
5	178	156	13
6	264	300	-32
7	448	422	28
8	299	327	-23
9	107	74	10
10	510	508	1
11	575	556	17
12	-40	64	-5
13	265	255	4
14	115	0	12
15	-133	16	-16
16	-84	14	-9
17	104	68	7
18	301	301	0
19	133	157	-7
20	337	338	0
21	86	128	-9
22	172	191	-6
23	146	170	-7
24	94	137	-9

7 1 L

1	305	313	-7
2	114	117	-1
3	256	256	0
4	287	249	30
5	284	251	30
6	143	98	15
7	310	300	9
8	130	139	-3
9	-4	16	0
10	161	141	6
11	239	228	4
12	73	56	2
13	181	87	23
14	72	3	4
15	68	122	-9
16	127	93	8
17	167	165	0
18	53	46	0
19	231	192	19
20	57	55	0
21	-59	28	-4
22	154	120	9
23	174	155	6
24	115	22	12
25	175	100	19
26	11	121	-12

9 1 L

1	714	723	-11
2	516	526	-10
3	856	838	20
4	1410	1405	4
5	549	547	2
6	1022	1026	-4
7	26	11	0
8	730	718	11
9	402	387	12
10	602	600	1
11	512	479	25
12	190	135	15
13	555	563	-6
14	-128	173	-41
15	277	292	-7
16	320	357	-20
17	113	69	8
18	732	744	-10
19	198	196	0
20	501	529	-22
21	136	93	10
22	225	278	-22
23	237	211	11
24	104	142	-8
25	272	268	1

11 1 L

1	581	581	0
2	450	444	5
3	398	406	-7
4	411	404	6
5	95	92	0
6	1061	1081	-19
7	421	446	-12
8	1060	1084	-14
9	490	481	4
10	345	321	9
11	306	260	17
12	222	213	2
13	519	522	-1
14	317	324	-2
15	571	562	4
16	624	649	-20
17	374	395	-13
18	309	314	-2
19	-55	10	-2
20	290	275	5
21	111	57	6
22	331	344	-4
23	210	198	3
24	-65	52	-4
25	173	124	9

13 1 L

1	143	27	13
2	192	97	18
3	125	105	2
4	114	64	5
5	200	135	13
6	518	540	-11
7	563	567	-2
8	506	495	6
9	211	196	4
10	126	52	9
11	132	65	9
12	-91	39	-6
13	-144	105	-19
14	194	214	-4
15	455	464	-4
16	496	509	-10
17	163	127	9
18	-58	22	-3
19	-88	17	-6
20	118	5	10
21	-171	55	-19
22	-71	61	-5
23	-105	53	-8
24	151	27	14

15 1 L

1	553	549	2
2	327	355	-11

3	343	353	-3	13	227	50	28					
4	705	759	-33	14	98	37	4	1	94	193	-11	
5	312	334	-8	15	300	262	10	2	108	89	1	
6	450	465	-7	16	265	231	13	3	88	73	1	
7	223	244	-6	17	82	50	3	4	109	26	5	
8	340	319	8	18	165	172	-1					
9	102	114	-1	19	94	65	3		0 2 L			
10	536	512	12									
11	519	526	-3		21 1 L			0	1380	1437	-37	
12	92	42	4					1	219	199	11	
13	272	245	8	1	304	315	-3	2	296	285	8	
14	-100	10	-6	2	262	238	6	3	1352	1376	-15	
15	200	70	22	3	358	342	5	4	1027	1039	-9	
16	108	66	6	4	439	452	-5	5	888	885	2	
17	131	51	13	5	64	50	0	6	469	471	-2	
18	487	457	20	6	639	653	-7	7	2039	2003	23	
19	-29	59	-3	7	242	241	0	8	667	604	71	
20	379	424	-17	8	607	595	5	9	1471	1441	24	
21	216	178	10	9	314	315	0	10	969	935	33	
22	199	165	7	10	161	233	-13	11	662	674	-12	
23	147	126	3	11	36	131	-7	12	259	133	33	
				12	122	90	3	13	723	717	3	
	17 1 L			13	391	351	13	14	1344	1323	11	
				14	217	221	0	15	525	626	-51	
1	480	502	-11	15	260	304	-10	16	-142	67	-25	
2	346	327	7	16	417	404	7	17	746	746	0	
3	223	203	5	17	222	191	9	18	241	232	3	
4	363	361	0					19	437	457	-11	
5	169	33	19		23 1 L			20	188	125	15	
6	645	643	1					21	664	656	5	
7	182	145	7	1	354	368	-4	22	130	83	6	
8	655	644	6	2	272	291	-5	23	196	136	13	
9	159	201	-8	3	477	414	26	24	367	338	11	
10	317	351	-11	4	643	640	1	25	69	131	-7	
11	450	420	13	5	298	269	7	26	171	73	15	
12	-124	128	-17	6	537	500	16					
13	297	322	-8	7	-98	99	-9		2 2 L			
14	230	134	21	8	400	360	14					
15	399	350	18	9	170	218	-8	0	647	681	-45	
16	358	341	9	10	319	320	0	1	91	33	14	
17	235	184	18	11	214	263	-9	2	185	9	66	
18	175	183	-2	12	-122	108	-11	3	1007	989	20	
19	177	163	3	13	317	317	0	4	828	821	8	
20	310	319	-3	14	-94	62	-5	5	593	590	4	
21	-66	137	-13					6	545	543	2	
					25 1 L			7	543	573	-34	
	19 1 L							8	1098	1081	17	
				1	175	134	5	9	271	225	25	
1	-186	48	-21	2	-105	17	-5	10	481	468	10	
2	80	62	1	3	192	116	11	11	469	438	23	
3	253	244	2	4	-92	153	-14	12	214	150	21	
4	127	249	-24	5	170	204	-5	13	176	105	18	
5	232	154	18	6	120	35	6	14	92	77	2	
6	343	323	7	7	201	13	20	15	192	201	-3	
7	176	221	-10	8	123	221	-14	16	308	284	16	
8	132	175	-7	9	103	71	2	17	519	513	4	
9	115	91	2	10	187	53	16	18	431	418	10	
10	167	96	10	11	-92	64	-5	19	290	309	-11	
11	65	7	2					20	412	420	-5	
12	-128	3	-8		27 1 L			21	379	385	-4	

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22	228	199	11	22	308	313	-2	24	163	160	0
23	108	56	8	23	423	424	0				
24	320	265	27	24	86	127	-7		12 2 L		
25	91	68	3	25	211	104	31				
26	49	1	2	26	-50	132	-16	0	661	685	-14
								1	333	306	10
	4 2 L				8 2 L			2	365	355	3
								3	1324	1353	-16
0	564	571	-9	0	147	70	20	4	1032	1043	-6
1	712	686	32	1	554	531	22	5	827	831	-2
2	1151	1152	-1	2	810	825	-16	6	520	471	26
3	572	523	58	3	479	465	15	7	962	966	-2
4	153	35	46	4	214	181	15	8	340	354	-5
5	832	808	28	5	1001	1010	-8	9	457	490	-16
6	408	409	-1	6	460	463	-2	10	537	531	3
7	127	88	14	7	774	771	2	11	512	480	16
8	430	429	0	8	889	886	2	12	138	34	11
9	552	548	3	9	1136	1132	3	13	286	207	24
10	393	370	15	10	255	108	48	14	433	431	0
11	91	41	6	11	139	107	6	15	193	128	12
12	596	567	23	12	597	591	4	16	-63	29	-4
13	246	162	31	13	147	87	13	17	641	643	-1
14	316	339	-12	14	143	165	-6	18	160	153	1
15	238	263	-10	15	590	604	-11	19	638	675	-19
16	468	442	23	16	540	537	2	20	501	555	-24
17	102	108	-1	17	270	284	-7	21	648	667	-9
18	346	324	12	18	310	302	4	22	132	128	0
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20	106	23	11	20	244	223	9				
21	181	185	-1	21	288	287	0		14 2 L		
22	219	214	1	22	294	263	14				
23	-44	130	-16	23	227	222	1	0	780	791	-6
24	-32	75	-5	24	170	44	26	1	186	241	-13
25	224	192	12	25	151	76	15	2	479	489	-5
26	360	361	0					3	236	278	-12
					10 2 L			4	184	139	9
	6 2 L							5	410	458	-22
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1	321	337	-14	2	657	648	8	8	247	185	17
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8	336	311	16	9	171	108	16	15	141	207	-12
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15	445	441	2	17	199	202	-1	22	171	86	14
16	426	403	18	18	289	289	0				
17	408	420	-8	19	198	173	9		16 2 L		
18	-81	2	-7	20	77	17	5				
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20	420	389	21	22	178	149	8	1	83	76	0
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9	222	192	7	0	-18	174	-14	18	-92	13	-8
10	246	223	6	1	182	67	14	19	111	24	12
11	-113	142	-17	2	108	129	-2	20	141	36	19
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16	270	229	16	7	18	93	-3	25	190	152	10
17	109	117	-1	8	301	270	8				
18	237	146	28	9	344	258	23		3 3 L		
19	-90	48	-6	10	230	148	14				
20	297	321	-8	11	157	9	11	1	1487	1477	7
21	-128	159	-22	12	260	197	12	2	224	178	21
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	18 2 L			14	56	97	-2	4	392	367	18
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1	265	235	8		24 2 L			7	239	145	34
2	485	490	-2					8	241	259	-7
3	195	198	0	0	434	393	13	9	502	434	50
4	283	246	11	1	165	16	13	10	424	396	18
5	704	727	-12	2	-95	123	-11	11	547	540	5
6	379	347	13	3	294	313	-5	12	180	193	-4
7	354	358	-1	4	293	262	7	13	678	658	17
8	201	131	13	5	220	239	-3	14	285	252	15
9	421	403	7	6	266	201	14	15	650	656	-5
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11	-94	71	-7	8	-165	91	-14	17	362	364	-1
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15	273	243	7					21	320	312	4
16	262	263	0		26 2 L			22	150	15	22
17	212	249	-12					23	478	462	11
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19	340	362	-7	1	142	4	9	25	368	399	-16
				2	175	22	14				
	20 2 L			3	450	444	2		5 3 L		
				4	307	264	10				
0	70	7	2	5	367	384	-5	1	318	304	8
1	469	451	7					2	553	522	27
2	667	644	12		1 3 L			3	488	466	18
3	542	555	-6					4	137	111	6
4	121	94	3	1	567	550	17	5	301	267	18
5	803	819	-8	2	216	170	22	6	176	77	24
6	223	227	0	3	431	401	25	7	172	97	18
7	567	557	4	4	165	23	32	8	279	267	5
8	445	455	-3	5	301	242	34	9	350	295	30
9	753	742	5	6	367	342	17	10	137	132	1
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12	458	436	8	9	617	603	11	13	466	434	22
13	-103	47	-6	10	517	507	7	14	114	151	-8
14	-111	89	-9	11	1075	1079	-3	15	427	423	3

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16	85	70	1	22	88	110	-3	7	107	110	0
17	216	202	6	23	218	246	-10	8	126	189	-11
18	114	56	10					9	407	414	-2
19	-67	74	-9		11 3 L			10	117	28	7
20	238	245	-2					11	651	642	4
21	-80	45	-7	1	1236	1232	2	12	59	64	0
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23	35	13	0	3	659	708	-27	14	-118	49	-7
24	178	184	-1	4	204	238	-9	15	383	462	-26
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	7 3 L			6	168	218	-11	17	195	186	2
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2	287	265	10	9	351	362	-4	20	194	234	-9
3	213	163	17	10	326	258	24				
4	59	70	-1	11	451	422	12		17 3 L		
5	194	68	29	12	187	103	14				
6	190	43	32	13	524	521	1	1	720	731	-6
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8	252	193	23	15	444	439	2	3	527	531	-1
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15	189	148	15	22	59	62	0	10	235	215	4
16	-40	56	-5					11	362	339	7
17	-96	96	-15		13 3 L			12	81	96	-1
18	-72	23	-5					13	412	377	11
19	-48	18	-2	1	609	652	-23	14	240	159	15
20	131	165	-8	2	540	532	4	15	455	422	12
21	147	83	14	3	207	190	4	16	-34	40	-2
22	-72	6	-4	4	118	71	5	17	279	209	26
23	127	31	13	5	203	2	26	18	156	128	5
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	9 3 L			8	135	92	5				
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12	132	169	-9	21	342	337	1	13	186	169	2
13	942	930	10					14	-113	86	-9
14	188	88	23		15 3 L			15	19	102	-4
15	560	550	7					16	118	67	7
16	220	238	-6	1	391	374	6				
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20	191	122	21	5	303	276	9	2	76	156	-8
21	116	128	-2	6	168	131	6	3	412	436	-8

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5	-32	137	-8
6	196	155	6
7	215	74	20
8	-205	20	-18
9	240	324	-18
10	-67	34	-2
11	412	397	4
12	-92	23	-3
13	412	417	-1
14	150	13	10

23 3 L

1	448	425	8
2	209	198	2
3	458	397	22
4	123	107	1
5	206	193	2
6	280	160	25
7	-131	44	-8
8	103	76	2
9	355	388	-9
10	81	51	1

25 3 L

1	245	179	12
2	204	1	19
3	-278	134	-35
4	-108	74	-7

0 4 L

0	717	715	1
1	-96	77	-10
2	787	839	-35
3	414	425	-5
4	305	241	24
5	1077	1092	-9
6	549	560	-6
7	971	1003	-21
8	283	292	-3
9	426	432	-3
10	491	485	3
11	275	226	16
12	686	683	1
13	117	158	-7
14	463	446	8
15	443	464	-15
16	645	693	-39
17	661	675	-11
18	367	388	-12
19	422	391	15
20	186	241	-14
21	280	205	24
22	223	191	8
23	182	233	-13

2 4 L

0	553	538	12
1	223	161	23
2	249	257	-3
3	270	238	16
4	440	414	19
5	139	144	-1
6	525	555	-25
7	49	98	-7
8	119	163	-12
9	330	337	-4
10	339	332	4
11	158	146	3
12	204	247	-16
13	-18	41	-1
14	347	352	-2
15	76	41	4
16	104	147	-11
17	68	45	2
18	207	201	2
19	189	199	-3
20	128	53	13
21	266	187	35
22	168	148	6
23	100	90	1

4 4 L

0	341	362	-12
1	67	28	3
2	274	191	37
3	240	226	6
4	246	283	-18
5	418	420	-1
6	341	343	-1
7	351	345	3
8	159	145	4
9	137	122	3
10	217	214	1
11	167	111	14
12	206	184	7
13	42	21	1
14	218	234	-6
15	117	92	6
16	23	63	-3
17	264	253	5
18	100	131	-6
19	162	169	-2
20	-55	16	-3
21	96	88	1
22	118	111	1
23	-120	78	-18

6 4 L

0	633	683	-45
1	219	238	-8
2	645	649	-3
3	400	393	4
4	304	324	-12
5	90	133	-9
6	-72	3	-5
7	386	332	36
8	259	235	11
9	505	524	-14
10	474	473	0
11	264	285	-9
12	558	543	11
13	100	91	1
14	415	441	-16
15	-75	1	-6
16	332	304	16
17	-81	0	-6
18	140	99	8
19	270	243	12
20	108	89	3
21	349	349	0
22	171	193	-7

8 4 L

0	494	523	-23
1	-153	30	-22
2	527	515	9
3	356	342	8
4	202	218	-6
5	625	667	-36
6	129	165	-10
7	648	660	-10
8	184	215	-10
9	251	262	-4
10	311	319	-4
11	171	184	-3
12	399	436	-22
13	-167	66	-26
14	345	322	11
15	289	270	10
16	323	359	-21
17	437	460	-14
18	237	181	23
19	290	243	22
20	121	108	2
21	166	153	3
22	111	149	-8

10 4 L

0	141	57	15
1	-90	73	-12
2	133	161	-7
3	134	23	17
4	37	99	-7
5	64	55	1
6	367	394	-16
7	127	107	4
8	-61	36	-4
9	169	108	15
10	-184	37	-28
11	109	21	9
12	134	122	2

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13	-136	13	-14	2	71	33	2	6	224	176	8
14	100	14	7	3	-83	0	-3	7	128	33	7
15	71	90	-2	4	152	139	2	8	-91	59	-5
16	270	262	3	5	-93	77	-8				
17	72	33	4	6	205	279	-17		1 5 L		
18	219	218	0	7	152	13	12				
19	-128	28	-14	8	209	0	24	1	464	439	16
20	68	92	-3	9	109	12	6	2	742	744	-1
21	146	46	19	10	174	26	16	3	264	246	7
				11	156	6	13	4	372	324	27
	12 4 L			12	-86	9	-3	5	164	26	22
				13	-245	35	-27	6	366	336	16
0	673	691	-10	14	122	44	6	7	169	22	23
1	164	58	15	15	50	1	1	8	465	426	25
2	429	437	-3	16	153	159	-1	9	95	51	5
3	362	417	-22	17	-131	8	-13	10	193	91	16
4	508	524	-8					11	138	62	11
5	845	856	-6		18 4 L			12	216	121	24
6	476	490	-7					13	-29	9	0
7	672	641	17	0	415	430	-5	14	146	60	12
8	254	242	3	1	135	129	0	15	153	11	23
9	323	346	-8	2	312	327	-4	16	242	223	7
10	467	451	7	3	196	237	-8	17	94	84	1
11	125	185	-9	4	272	231	10	18	189	167	6
12	436	410	11	5	-80	112	-9	19	97	83	2
13	198	70	18	6	230	119	20	20	+57	481	-14
14	466	458	3	7	132	204	-11				
15	243	258	-5	8	-127	152	-18		3 5 L		
16	-45	25	-2	9	275	288	-3				
17	539	476	40	10	262	259	0	1	180	65	23
18	215	180	11	11	242	162	16	2	126	136	-2
19	335	378	-15	12	263	291	-6	3	-106	25	-9
20	-188	19	-21	13	169	48	13	4	726	722	3
				14	228	248	-4	5	213	95	31
	14 4 L			15	-38	6	-1	6	779	768	9
								7	-86	7	-6
0	406	434	-11		20 4 L			8	715	721	-4
1	84	209	-20					9	213	136	21
2	498	520	-11	0	443	449	-2	10	654	643	8
3	174	198	-5	1	97	13	4	11	204	149	14
4	-142	89	-16	2	395	394	0	12	126	2	12
5	157	60	13	3	308	307	0	13	223	168	15
6	334	373	-13	4	288	284	1	14	260	284	-8
7	219	219	0	5	629	613	7	15	118	118	0
8	-48	162	-15	6	138	111	3	16	314	318	-1
9	444	403	18	7	529	532	-1	17	84	+5	4
10	305	308	0	8	276	162	24	18	481	479	1
11	266	173	22	9	223	225	0	19	120	121	0
12	423	418	1	10	310	319	-2	20	310	265	21
13	-158	25	-12	11	243	158	16				
14	297	289	2	12	314	354	-10		5 5 L		
15	-21	34	-1								
16	466	455	6		22 4 L			1	122	42	10
17	75	39	3					2	196	167	8
18	303	285	7	0	-34	95	-4	3	159	36	20
				1	-112	32	-6	4	371	364	3
	16 4 L			2	139	133	0	5	166	25	22
				3	-129	14	-7	6	571	567	2
0	102	95	0	4	158	28	11	7	48	29	1
1	90	12	4	5	-56	69	-3	8	287	292	-2

9	124	149	-5	3	200	20	22	7	34	10	0
10	88	54	3	4	505	530	-10	8	387	426	-12
11	222	183	11	5	-120	78	-10	9	172	34	12
12	238	231	2	6	466	501	-13	10	299	327	-7
13	169	93	13	7	173	8	15	11	153	43	9
14	64	65	0	8	604	616	-5				
15	131	23	15	9	106	219	-16		19 5 L		
16	295	287	3	10	628	615	6				
17	-89	56	-8	11	323	258	16	1	156	131	3
18	281	254	12	12	103	89	1	2	236	190	8
19	-112	37	-11	13	287	222	15	3	-159	34	-11
20	223	174	16	14	354	331	6	4	142	83	5
				15	117	103	2	5	124	9	6
	7 5 L			16	210	187	6	6	150	39	9
				17	121	15	11	7	-70	0	-2
1	210	189	6					8	226	175	9
2	172	159	3		13 5 L						
3	-123	62	-14						0 6 L		
4	186	126	14	1	94	53	2				
5	161	35	20	2	126	26	7	0	615	614	0
6	286	268	7	3	31	24	0	1	245	203	10
7	74	14	4	4	128	125	0	2	885	899	-7
8	116	36	9	5	102	45	3	3	-89	102	-10
9	208	83	27	6	172	20	15	4	634	632	1
10	97	4	7	7	109	34	5	5	225	284	-16
11	135	152	-3	8	242	239	0	6	110	91	2
12	193	113	17	9	249	280	-7	7	340	318	7
13	58	58	0	10	392	385	2	8	130	161	-4
14	95	55	3	11	334	344	-2	9	145	213	-12
15	101	23	8	12	209	237	-5	10	402	360	15
16	92	128	-6	13	301	246	12	11	164	82	10
17	92	13	6	14	262	293	-6	12	548	511	16
18	115	112	0	15	80	75	0	13	-124	71	-9
19	-88	60	-9	16	96	45	5	14	335	351	-4
								15	116	173	-12
	9 5 L				15 5 L			16	362	374	-5
1	253	275	-8	1	85	103	-1		2 6 L		
2	585	597	-8	2	368	350	5				
3	170	185	-3	3	-69	120	-8	0	348	355	-3
4	600	602	-1	4	427	408	6	1	191	249	-20
5	146	16	15	5	-45	27	-1	2	146	29	18
6	703	678	18	6	577	579	0	3	369	363	3
7	113	25	9	7	168	31	12	4	-136	8	-14
8	601	623	-14	8	382	331	15	5	88	184	-19
9	121	36	9	9	214	166	8	6	-161	164	-37
10	306	281	9	10	149	41	9	7	155	124	6
11	202	35	28	11	208	173	6	8	135	185	-11
12	216	150	15	12	322	242	20	9	-104	47	-9
13	192	32	24	13	-104	89	-7	10	290	249	16
14	163	101	10	14	157	50	9	11	77	29	3
15	24	52	-1					12	246	221	8
16	344	352	-4		17 5 L			13	142	33	14
17	110	100	1					14	343	340	1
18	394	373	11	1	81	68	0	15	24	38	0
				2	147	87	6	16	124	109	3
	11 5 L			3	-134	19	-7				
				4	422	431	-3		4 6 L		
1	114	7	6	5	192	33	16				
2	-62	139	-11	6	529	493	13	0	222	269	-16

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1	78	57	2
2	217	138	23
3	-89	114	-16
4	52	124	-9
5	153	126	5
6	169	65	20
7	85	43	4
8	271	251	7
9	140	84	9
10	264	215	16
11	88	1	5
12	190	198	-2
13	146	131	2
14	313	335	-8
15	-41	18	-2
16	116	127	-2

6 6 L

0	540	522	11
1	169	193	-6
2	421	394	14
3	265	333	-28
4	160	170	-2
5	257	268	-3
6	129	105	4
7	293	316	-10
8	125	2	12
9	381	346	16
10	281	286	-1
11	-105	80	-11
12	392	369	10
13	258	213	14
14	240	218	6
15	214	210	1

8 6 L

0	413	425	-6
1	128	91	6
2	535	527	4
3	-124	16	-10
4	372	380	-3
5	227	195	9
6	141	22	14
7	190	185	1
8	189	175	3
9	-40	103	-8
10	270	255	5
11	205	57	29
12	344	337	2
13	88	7	5
14	310	306	1

10 6 L

0	-58	77	-6
1	-103	86	-12
2	177	218	-10
3	102	82	2
4	87	122	-5
5	127	11	11
6	123	57	8
7	32	81	-3
8	-134	107	-18
9	184	160	5
10	169	8	20
11	-52	28	-2
12	91	59	3
13	88	155	-10

12 6 L

0	522	540	-7
1	-54	87	-5
2	320	356	-10
3	270	201	15
4	264	291	-6
5	124	242	-19
6	-155	89	-14
7	83	112	-2
8	472	436	13
9	167	121	6
10	468	434	12
11	137	15	8

14 6 L

0	338	352	-4
1	71	46	1
2	435	403	11
3	-59	133	-9
4	233	187	9
5	179	185	-1
6	127	24	7
7	288	301	-3
8	231	154	14
9	398	387	3

16 6 L

0	-54	3	-1
1	175	53	12
2	41	95	-3
3	147	87	6
4	130	33	7

1 7 L

1	210	245	-9
2	-108	104	-13
3	-109	91	-12
4	-148	35	-14
5	205	246	-11
6	366	368	0
7	263	238	7
8	295	321	-9
9	-89	82	-9

3 7 L

1	473	457	8
2	-127	72	-13
3	267	318	-17
4	318	312	2
5	107	23	7
6	112	146	-5
7	222	214	2
8	-137	95	-16
9	236	252	-4

5 7 L

1	263	242	6
2	-88	67	-7
3	279	313	-11
4	78	58	1
5	244	199	12
6	-114	8	-8
7	129	81	6
8	138	112	4

7 7 L

1	-76	72	-6
2	-102	13	-6
3	116	189	-13
4	169	51	16
5	122	39	8
6	203	127	16
7	144	161	-3

9 7 L

1	377	395	-7
2	67	120	-5
3	249	266	-4
4	-150	117	-20

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0 0 L

4	3320	3316	1
6	1998	1976	10
8	1683	1654	15
10	3289	3286	0
12	886	860	27
14	2924	2933	-2
16	1033	1042	-5
18	1798	1797	0
20	1483	1516	-17
22	-119	72	-13
24	1974	1989	-6
26	690	705	-7
28	1257	1300	-20
30	562	579	-7
32	619	621	0
34	680	651	13
36	391	398	-2
38	690	680	4
40	400	366	12

2 0 L

2	2423	2342	31
4	3998	3952	16
6	2856	2834	7
8	2289	2230	24
10	2977	2935	12
12	990	1006	-16
14	2237	2248	-4
16	1166	1170	-2
18	1533	1570	-19
20	1377	1374	1
22	1533	1556	-11
24	1036	1071	-19
26	528	508	9
28	968	972	-2
30	698	698	0
32	715	725	-4
34	848	834	6
36	491	487	1
38	564	571	-3
40	389	365	8

4 0 L

0	2422	2424	0
2	3569	3581	-3
4	2397	2360	15
6	2523	2472	19
8	2301	2273	11
10	1176	1194	-12
12	3027	2964	27
14	1487	1475	6
16	1782	1793	-5
18	1251	1272	-12
20	1164	1179	-9
22	1192	1215	-12
24	874	896	-13
26	1156	1169	-6
28	765	774	-4
30	865	857	4
32	818	790	14
34	380	357	7
36	645	628	7
38	475	492	-6
40	565	538	12

6 0 L

0	1970	1911	28
2	3823	3881	-14
4	1320	1308	7
6	2443	2417	10
8	2811	2815	-1
10	1627	1587	29
12	2348	2360	-4
14	700	678	15
16	2237	2245	-3
18	1288	1282	3
20	1189	1214	-14
22	1246	1226	11
24	651	685	-18
26	1461	1452	4
28	490	521	-14
30	878	848	15
32	575	538	17
34	703	718	-7
36	753	700	25
38	339	322	5
40	559	519	17

8 0 L

0	138	72	19
2	3700	3722	-6
4	1858	1831	13
6	2405	2414	-3
8	2455	2474	-10
10	1102	1087	14
12	2671	2654	6
14	904	898	4
16	1892	1910	-8
18	1097	1104	-4
20	1070	1060	5
22	1778	1806	-12
24	481	441	18
26	1122	1122	0
28	535	547	-5
30	903	893	5
32	751	755	-2
34	471	511	-15
36	680	650	14
38	383	388	-1
40	564	531	14

10 0 L

0	3205	3160	13
2	1894	1897	-1
4	2128	2133	-2
6	1902	1904	-1
8	1690	1681	6
10	1580	1568	6
12	1965	1988	-10
14	1734	1751	-8
16	1290	1299	-5
18	1241	1259	-10
20	1172	1192	-11
22	694	714	-10
24	1165	1183	-9
26	868	903	-18
28	890	891	0
30	776	728	24
32	732	702	14
34	388	392	-1
36	527	527	0
38	593	559	15

12 0 L

0	2908	2939	-14
2	886	847	39
4	2581	2572	4
6	1821	1820	0
8	1533	1533	0
10	3068	3133	-19
12	250	213	14
14	2121	2121	0
16	872	874	-1
18	1513	1526	-6
20	1315	1339	-12
22	766	774	-4
24	1319	1298	10
26	413	411	0
28	1002	985	8
30	532	529	1
32	443	451	-3
34	1083	1065	8
36	328	374	-14
38	557	519	16

14 0 L

0	2892	2958	-22
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4	2330	2335	-1
6	1535	1558	-12
8	1134	1125	5
10	1541	1542	0
12	1468	1477	-4
14	2113	2154	-16
16	710	723	-8
18	1174	1214	-21
20	1013	1048	-18
22	572	618	-23
24	1277	1294	-8
26	524	518	2

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28	1006	1022	-8	14	434	465	-13	10	1332	1336	-1
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32	809	810	0	18	685	698	-6	14	1252	1276	-11
34	206	272	-14	20	722	725	-1	16	415	443	-11
36	407	406	0	22	1247	1260	-6	18	832	830	1
38	643	632	5	24	262	370	-33	20	709	707	0
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	16	0 L		28	389	410	-7	24	672	672	0
				30	703	723	-9	26	219	252	-7
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2	1619	1642	-11	34	191	258	-15	30	466	440	10
4	1647	1673	-13								
6	1568	1586	-9		22	0 L			28	0 L	
8	1535	1571	-18								
10	1677	1703	-12	0	814	829	-9	0	1612	1598	6
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14	1216	1212	2	4	1070	1083	-7	4	1012	982	16
16	1087	1110	-13	6	1196	1203	-3	6	775	791	-8
18	1127	1149	-12	8	1217	1222	-2	8	749	745	2
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22	1119	1127	-4	12	884	877	3	12	672	669	1
24	730	748	-9	14	778	786	-4	14	980	983	-1
26	726	701	13	16	1059	1079	-10	16	607	594	6
28	712	707	2	18	846	849	-1	18	796	791	2
30	608	618	-4	20	864	860	2	20	716	724	-3
32	533	532	0	22	892	898	-2	22	202	285	-18
34	693	694	0	24	538	555	-7	24	804	797	3
36	540	509	14	26	684	710	-12	26	522	500	9
				28	584	550	15	28	661	626	16
	18	0 L		30	656	611	20	30	408	422	-5
				32	474	414	23				
0	1119	1166	-30	34	657	623	16		30	0 L	
2	2020	2033	-5								
4	909	914	-3		24	0 L		0	515	533	-7
6	1414	1410	2					2	1022	1022	0
8	1642	1659	-8	0	2163	2177	-5	4	704	669	17
10	899	911	-7	2	483	484	0	6	810	818	-4
12	1663	1701	-18	4	1205	1237	-17	8	927	905	11
14	656	633	13	6	939	973	-19	10	728	708	9
16	1487	1515	-13	8	821	818	1	12	759	770	-5
18	930	945	-8	10	1213	1250	-19	14	515	532	-7
20	852	874	-11	12	680	694	-7	16	828	791	18
22	806	819	-7	14	1303	1292	5	18	653	636	7
24	630	634	-2	16	632	657	-12	20	524	557	-13
26	1083	1071	6	18	891	895	-2	22	715	699	7
28	535	515	8	20	845	868	-12	24	451	451	0
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32	550	529	9	24	1085	1070	7	28	376	397	-7
34	522	509	5	26	535	529	2				
36	562	545	10	28	715	706	4		32	0 L	
				30	490	464	10				
	20	0 L		32	504	492	5	0	-119	38	-8
								2	1271	1256	7
0	42	165	-18		26	0 L		4	544	531	6
2	2222	2219	1					6	791	776	7
4	892	917	-16	0	958	994	-18	8	879	861	8
6	1401	1412	-5	2	602	607	-2	10	79	231	-24
8	1477	1490	-6	4	1445	1459	-6	12	1225	1194	14
10	235	272	-12	6	930	958	-15	14	321	309	3
12	2170	2208	-15	8	733	723	5	16	856	834	10

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18	467	479	-4	7	136	144	-3	11	573	567	4
20	518	466	23	8	243	231	7	12	189	68	26
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6	708	684	11	17	-14	205	-29	21	82	132	-10
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12	830	809	9	20	357	427	-43	24	181	163	5
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	36 0 L				3 1 L			3	293	278	15
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6	605	601	1	4	446	505	-58	8	148	136	3
8	548	552	-1	5	214	161	29	9	-37	4	-1
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12	315	315	0	7	505	461	39	11	289	256	13
14	623	627	-1	8	1517	1483	28	12	-128	52	-14
16	476	514	-15	9	560	555	6	13	0	70	-3
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	38 0 L			12	277	273	1	16	70	99	-5
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6	476	464	4					4	1432	1424	6
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	1 1 L			3	122	137	-8	7	31	18	0
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1	351	315	35	5	146	150	-2	9	405	384	11
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3	1538	1518	11	7	467	439	33	11	531	524	4
4	2293	2255	15	8	334	349	-15	12	173	132	9
5	1249	1211	26	9	121	91	10	13	542	574	-20
6	1007	982	28	10	527	529	-1	14	198	191	2

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15	331	333	-1	19	-141	51	-14	23	280	184	26	
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22	297	316	-6					4	244	289	-16	
23	172	236	-15		15 1 L			5	105	146	-7	
24	91	170	-11					6	346	370	-11	
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	11 1 L			3	377	372	2	9	159	124	7	
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13	534	534	0	17	-255	16	-41					
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17	372	405	-16	21	168	174	-1	2	208	253	-13	
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23	267	206	17		17 1 L			8	615	627	-6	
24	109	60	5					9	309	308	0	
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	13 1 L			3	227	222	2	12	116	93	3	
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2	-85	95	-12	6	686	687	0	15	350	377	-10	
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16	530	541	-6	20	364	374	-3	6	585	555	15	
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9	197	231	-8	9	1498	1457	23	11	62	66	0
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	25 1 L			20	-98	184	-26	22	347	287	32
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6	-86	73	-7		2 2 L			0	140	7	34
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1	218	219	0	11	502	478	15	13	374	386	-6
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	29 1 L			23	-159	35	-21	25	161	88	15
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1	-67	110	-10	5	120	57	6	4	148	108	8
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8	411	352	24	4	143	20	19	11	432	419	7
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6	277	241	10					4	181	70	22
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3	263	262	0	2	557	533	16	8	173	117	12
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18	225	196	7				
19	-85	19	-4		17 3 L		
20	-56	104	-8				
21	421	403	7	1	780	796	-10
22	196	71	19	2	-43	37	-2
23	603	588	7	3	588	581	3
24	297	302	-1	4	162	218	-14
25	404	398	2	5	296	258	13
				6	-177	122	-30
	13 3 L			7	135	109	4
				8	237	210	7
1	599	652	-31	9	312	286	9
2	558	568	-6	10	321	253	25
3	246	192	16	11	375	369	2
4	177	81	18	12	-101	108	-13
5	95	17	8	13	462	455	3
6	132	73	13	14	106	177	-11
7	103	38	9	15	465	482	-7
8	172	95	22	16	81	41	2
9	70	42	3	17	327	267	19
10	223	101	30	18	-74	142	-13
11	115	55	7	19	-144	34	-11
12	177	55	21	20	204	76	22
13	-43	29	-1	21	236	188	10

19 3 L

1	334	346	-4
2	146	177	-6
3	106	155	-7
4	-76	5	-3
5	-79	49	-5
6	206	139	14
7	58	10	2
8	183	64	18
9	146	166	-3
10	58	118	-6
11	381	326	20
12	150	131	3
13	273	224	14
14	162	102	9
15	137	107	4
16	-41	80	-4
17	226	56	29
18	-110	34	-7
19	-105	12	-6

21 3 L

1	711	784	-38
2	204	183	4
3	466	471	-2
4	85	99	-1
5	-115	152	-20
6	199	175	5
7	145	86	7
8	-75	34	-4
9	285	336	-15
10	187	51	18
11	449	459	-4
12	48	23	1
13	430	448	-7
14	62	27	1
15	263	315	-14
16	177	97	13
17	230	190	8

23 3 L

1	492	491	0
2	213	222	-2
3	388	437	-19
4	179	102	12
5	205	227	-4
6	208	170	7
7	99	69	2
8	66	75	0
9	487	442	20
10	166	86	11
11	678	675	1
12	119	103	1
13	638	641	-1
14	93	76	1

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25 3 L

1	233	228	1
2	33	14	0
3	49	168	-13
4	127	87	4
5	-219	54	-26
6	96	9	5
7	-53	7	-1
8	154	167	-2
9	93	86	0
10	289	281	2
11	136	214	-14

27 3 L

1	339	311	8
2	-43	5	-1
3	283	218	17
4	133	84	5

0 4 L

0	730	749	-13
1	126	63	10
2	852	878	-18
3	502	499	1
4	219	238	-6
5	1122	1146	-22
6	576	570	4
7	1061	1078	-11
8	307	300	3
9	435	444	-5
10	520	519	0
11	258	263	-2
12	754	743	10
13	31	127	-16
14	463	495	-18
15	486	493	-4
16	743	756	-8
17	744	769	-15
18	400	425	-11
19	423	449	-12
20	276	265	3
21	242	265	-6
22	179	231	-11
23	210	260	-12
24	325	326	0

2 4 L

0	558	549	5
1	235	146	28
2	259	270	-4
3	250	273	-9
4	426	434	-4
5	147	130	3
6	549	579	-19
7	111	151	-8
8	180	178	0
9	342	344	-1
10	347	347	0
11	188	174	5
12	271	270	0
13	62	67	0
14	398	379	14
15	-48	34	-3
16	132	142	-2
17	-66	6	-4
18	204	212	-3
19	220	221	0
20	83	60	3
21	234	233	0
22	181	174	2
23	142	95	9
24	149	166	-4

4 4 L

0	338	377	-18
1	76	1	4
2	227	194	11
3	228	211	6
4	294	292	0
5	463	460	1
6	336	352	-7
7	362	342	10
8	148	143	1
9	164	151	4
10	232	230	1
11	38	94	-8
12	206	199	3
13	101	32	10
14	210	257	-22
15	124	132	-2
16	100	68	5
17	277	273	1
18	105	137	-6
19	215	208	2
20	40	20	1
21	-89	89	-13
22	-111	128	-24
23	96	98	0
24	158	119	8

6 4 L

0	686	717	-21
1	231	278	-17
2	682	671	7
3	400	397	1
4	320	354	-17
5	187	173	4
6	110	6	11
7	375	350	13
8	279	252	15
9	583	589	-5
10	500	504	-3
11	308	281	16
12	566	581	-13
13	136	88	12
14	466	487	-15
15	50	37	1
16	361	346	9
17	-173	10	-26
18	92	121	-5
19	313	307	3
20	-148	106	-27
21	430	399	18
22	228	226	0
23	-59	149	-20
24	225	275	-18

8 4 L

0	543	554	-7
1	-81	59	-8
2	499	546	-29
3	352	363	-5
4	279	230	20
5	713	758	-30
6	109	178	-22
7	660	683	-21
8	252	219	17
9	326	309	10
10	345	354	-5
11	210	186	7
12	486	481	3
13	97	77	2
14	395	369	12
15	288	319	-11
16	365	401	-16
17	528	510	9
18	268	202	19
19	335	314	7
20	100	127	-3
21	200	179	4
22	138	179	-7
23	80	186	-14
24	290	217	20

10 4 L

0	30	53	-2
1	63	53	1
2	131	176	-15
3	110	52	11
4	147	110	11
5	28	30	0
6	372	416	-31
7	97	102	-1
8	78	34	5
9	-101	87	-13
10	-76	40	-5
11	139	40	14
12	141	137	0
13	117	9	10
14	174	16	22
15	-134	62	-14
16	234	297	-18

17	154	33	15
18	270	236	10
19	37	21	0
20	-230	113	-34
21	-142	65	-13
22	34	25	0
23	-150	18	-12

12 4 L

0	728	729	0
1	53	42	1
2	447	461	-10
3	437	456	-14
4	547	550	-2
5	908	897	10
6	521	529	-4
7	739	725	8
8	213	264	-16
9	373	352	10
10	486	488	-1
11	244	213	10
12	469	454	7
13	122	51	8
14	482	512	-14
15	341	305	14
16	-143	28	-13
17	610	576	17
18	197	194	0
19	433	422	4
20	110	5	7
21	202	203	0
22	234	241	-1

14 4 L

0	439	459	-10
1	172	209	-10
2	549	563	-8
3	218	255	-11
4	98	103	0
5	134	80	9
6	394	400	-3
7	264	282	-6
8	143	175	-7
9	458	435	11
10	318	328	-4
11	185	205	-4
12	455	463	-3
13	113	49	6
14	319	319	0
15	178	33	19
16	524	528	-1
17	69	4	2
18	320	328	-2
19	100	193	-15
20	152	154	0
21	259	298	-11

16 4 L

0	182	111	14
1	-25	20	0
2	-126	27	-11
3	148	36	15
4	172	148	5
5	76	78	0
6	313	308	1
7	43	9	1
8	149	10	15
9	146	8	15
10	94	43	4
11	69	25	2
12	-131	4	-10
13	116	17	8
14	-179	68	-21
15	190	8	23
16	-66	174	-18
17	49	28	0
18	164	134	5
19	76	23	3

18 4 L

0	415	463	-20
1	157	158	0
2	358	351	2
3	287	254	11
4	259	254	1
5	168	139	5
6	85	131	-6
7	227	191	9
8	154	168	-2
9	332	333	0
10	315	295	6
11	171	166	1
12	350	331	7
13	-116	52	-9
14	340	298	14
15	-134	19	-10
16	27	102	-5
17	-152	14	-13
18	166	2	16

20 4 L

0	491	510	-8
1	126	35	9
2	416	438	-9
3	344	324	7
4	275	318	-13
5	734	702	17
6	-129	128	-18
7	599	607	-4
8	245	184	16
9	275	280	-1
10	385	366	7
11	-20	167	-16
12	396	407	-4
13	88	59	2
14	378	362	5
15	309	284	7

22 4 L

0	107	101	0
1	-198	53	-24
2	93	152	-8
3	-23	34	0
4	-110	31	-7
5	59	21	1
6	255	210	12
7	-71	43	-4
8	-62	55	-4
9	101	102	0
10	137	42	10
11	-98	43	-6
12	167	105	10
13	-121	9	-8

24 4 L

0	274	251	6
1	-21	36	-1
2	272	291	-5
3	179	183	0
4	171	19	17
5	352	368	-5
6	264	283	-5
7	420	374	17
8	-143	137	-21

1 5 L

1	484	483	0
2	787	776	10
3	281	247	17
4	373	349	15
5	100	30	9
6	397	376	14
7	157	15	26
8	492	467	18
9	123	41	13
10	129	113	3
11	30	67	-3
12	216	132	27
13	122	18	13
14	110	74	5
15	131	14	14
16	317	261	25
17	172	85	18
18	266	207	21
19	87	88	0
20	555	543	7
21	252	286	-13
22	300	313	-5
23	253	257	-1

3 5 L

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1	193	57	36	11	191	158	7					
2	165	158	2	12	180	123	10	1	156	41	14	
3	37	9	1	13	148	69	10	2	-191	31	-21	
4	781	781	0	14	247	65	35	3	142	33	11	
5	162	99	17	15	177	23	18	4	48	129	-8	
6	843	836	6	16	237	140	22	5	-59	43	-3	
7	109	1	12	17	154	16	13	6	-123	32	-9	
8	778	785	-6	18	142	123	2	7	76	26	2	
9	234	158	30	19	145	61	9	8	285	247	11	
10	701	692	7	20	164	71	11	9	246	293	-13	
11	211	186	9	21	160	169	-1	10	383	411	-10	
12	185	5	33					11	342	383	-14	
13	275	198	32		9 5 L			12	290	276	4	
14	326	318	4					13	352	269	27	
15	197	132	18	1	320	314	2	14	336	325	3	
16	390	373	9	2	654	639	9	15	80	63	1	
17	133	47	12	3	-27	189	-22	16	-88	63	-6	
18	574	564	6	4	649	650	0	17	154	35	13	
19	151	117	7	5	121	18	10	18	-177	89	-19	
20	351	336	7	6	750	756	-3	19	-84	31	-4	
21	115	155	-7	7	60	15	2					
22	290	232	21	8	704	695	5		15 5 L			
				9	-64	24	-2					
	5 5 L			10	338	321	6	1	201	120	14	
				11	25	35	0	2	415	391	9	
1	125	38	14	12	199	170	6	3	80	136	-6	
2	211	184	10	13	136	41	10	4	449	449	0	
3	136	52	16	14	170	126	7	5	132	22	9	
4	420	406	10	15	80	69	0	6	606	631	-12	
5	61	30	2	16	425	422	1	7	146	20	12	
6	625	616	7	17	181	104	13	8	424	374	19	
7	-125	21	-15	18	487	450	16	9	112	164	-7	
8	375	331	28	19	-46	10	-1	10	-37	54	-2	
9	167	143	7	20	539	560	-8	11	262	182	19	
10	155	75	18	21	198	137	11	12	343	277	21	
11	225	187	14					13	121	93	3	
12	300	254	22		11 5 L			14	187	50	18	
13	156	93	13					15	128	40	8	
14	-38	63	-4	1	-90	22	-5	16	370	373	0	
15	161	35	20	2	102	169	-10	17	-120	87	-11	
16	347	332	7	3	167	1	18					
17	139	68	11	4	596	593	1		17 5 L			
18	332	302	14	5	63	85	-2					
19	-87	36	-6	6	573	554	9	1	147	57	10	
20	227	218	2	7	126	10	10	2	124	97	3	
21	107	69	5	8	690	682	4	3	145	14	11	
22	221	209	3	9	228	247	-4	4	478	493	-6	
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	7 5 L			11	391	326	25	6	597	578	9	
				12	166	108	9	7	-23	7	0	
1	262	217	14	13	331	267	20	8	506	498	3	
2	135	170	-7	14	327	374	-15	9	-69	50	-4	
3	142	57	12	15	-100	112	-12	10	417	380	14	
4	163	139	5	16	218	219	0	11	122	46	7	
5	-72	36	-4	17	96	13	5	12	111	51	5	
6	246	277	-10	18	393	413	-7	13	150	71	9	
7	156	11	17	19	211	78	21	14	174	138	6	
8	72	33	2	20	285	309	-6	15	128	73	5	
9	156	88	11									
10	115	8	9		13 5 L				19 5 L			

1	141	153	-1
2	196	227	-6
3	-63	56	-3
4	170	114	9
5	-16	9	0
6	58	57	0
7	184	1	18
8	248	207	10
9	-123	92	-12
10	160	188	-4
11	197	171	5
12	-150	44	-13
13	270	100	35

21 5 L

1	153	110	5
2	219	232	-3
3	-168	51	-15
4	375	372	1
5	161	48	13
6	386	367	6
7	-90	1	-4
8	480	459	8
9	234	156	15

23 5 L

1	164	199	-6

0 6 L

0	697	685	7
1	195	198	0
2	975	989	-8
3	141	109	6
4	691	701	-5
5	290	296	-2
6	65	85	-2
7	386	354	14
8	186	200	-3
9	197	238	-11
10	456	434	10
11	-104	102	-13
12	623	606	9
13	-111	65	-9
14	457	431	11
15	126	195	-13
16	428	435	-2
17	173	197	-4
18	-91	36	-5
19	110	3	7

2 6 L

0	381	404	-14
1	235	254	-9
2	-20	56	-3
3	416	387	20
4	146	3	23
5	118	204	-27
6	99	165	-16
7	169	125	12
8	238	210	11
9	-128	57	-18
10	272	283	-5
11	-144	32	-19
12	248	259	-4
13	-231	34	-43
14	393	385	4
15	103	38	8
16	69	137	-11
17	112	137	-5
18	152	136	3
19	260	259	0

4 6 L

0	306	295	5
1	125	58	12
2	117	158	-10
3	134	123	2
4	114	140	-6
5	146	133	3
6	-44	62	-5
7	-73	43	-6
8	307	278	14
9	30	88	-6
10	264	244	8
11	153	6	22
12	247	222	10
13	81	141	-11
14	363	374	-6
15	-99	23	-8
16	129	148	-4
17	-33	97	-9
18	37	1	1
19	160	96	13

6 6 L

0	599	602	-2
1	218	199	6
2	464	445	13
3	324	361	-21
4	178	189	-3
5	323	295	14
6	159	111	12
7	304	347	-23
8	97	10	9
9	381	387	-3
10	319	337	-9
11	168	94	18
12	460	439	13
13	201	230	-10
14	303	272	14
15	242	228	5
16	254	248	2
17	164	184	-5
18	181	241	-18

8 6 L

0	404	481	-31
1	-41	87	-5
2	581	597	-8
3	57	18	2
4	450	438	5
5	264	206	16
6	-58	17	-2
7	200	215	-3
8	263	205	17
9	196	113	16
10	312	318	-2
11	142	68	9
12	414	412	0
13	58	14	1
14	254	373	-35
15	131	105	3
16	349	284	23
17	81	140	-7

10 6 L

0	-133	67	-12
1	123	76	6
2	257	227	9
3	-182	85	-24
4	215	130	19
5	93	12	5
6	143	51	11
7	74	111	-4
8	73	129	-6
9	275	183	27
10	90	3	4
11	-139	31	-12
12	151	77	10
13	199	167	7
14	100	108	-1
15	-169	118	-24
16	220	28	28

12 6 L

0	593	617	-12
1	147	87	8
2	431	414	7
3	128	220	-17
4	392	330	26
5	232	273	-11
6	78	87	0
7	85	110	-2
8	537	511	12
9	219	129	19
10	531	497	15
11	124	29	9
12	469	481	-5
13	283	248	10
14	704	720	-8

15	-49	28	-1	4	-86	54	-8	4	112	56	5
				5	254	257	-1	5	20	57	-1
	14 6 L			6	396	412	-9	6	172	143	5
				7	224	255	-11	7	141	179	-6
0	482	413	30	8	341	369	-13	8	-72	50	-4
1	31	47	0	9	-118	90	-17	9	149	130	2
2	470	467	1	10	22	4	0	10	127	54	7
3	151	136	2	11	278	292	-5	11	-119	17	-7
4	223	219	1	12	95	83	1	12	-107	16	-6
5	94	200	-18	13	119	179	-13				
6	61	31	1	14	92	127	-5		9 7 L		
7	361	341	7								
8	127	163	-6		3 7 L			1	489	463	10
9	404	434	-11					2	-105	140	-16
10	186	167	3	1	526	523	2	3	221	328	-25
11	-192	91	-24	2	-42	102	-9	4	244	142	22
12	340	303	12	3	343	360	-8	5	198	258	-13
13	346	306	13	4	374	367	3	6	417	360	22
				5	-98	8	-8	7	-147	70	-14
	16 6 L			6	133	192	-14	8	346	358	-4
				7	167	234	-19	9	267	242	6
0	-112	28	-7	8	147	127	4	10	201	126	13
1	74	70	0	9	270	297	-10	11	430	402	10
2	204	83	22	10	223	249	-8				
3	154	104	7	11	331	384	-24		11 7 L		
4	-104	25	-6	12	83	48	3				
5	81	39	2	13	399	409	-5	1	445	410	14
6	228	48	31	14	-46	24	-2	2	-44	85	-5
7	-159	32	-15					3	79	166	-11
8	-114	134	-16		5 7 L			4	401	412	-3
9	149	89	8					5	155	106	7
10	97	59	3	1	263	281	-7	6	240	246	-1
11	113	5	7	2	-141	77	-19	7	72	139	-7
				3	349	359	-5	8	89	95	0
	18 6 L			4	-123	45	-13	9	182	176	1
				5	230	228	0				
0	305	357	-14	6	63	29	2		13 7 L		
1	170	147	3	7	-105	96	-15				
2	202	210	-1	8	130	137	-1	1	90	85	0
3	296	251	13	9	181	231	-15	2	-123	20	-8
4	147	96	7	10	-87	85	-11	3	74	144	-7
5	182	176	1	11	145	199	-13	4	390	339	17
6	120	91	3	12	70	67	0	5	314	253	16
7	108	182	-12	13	300	277	9	6	-69	155	-14
	1 7 L				7 7 L				0 8 L		
1	297	281	7	1	56	78	-1	0	-71	107	-8
2	109	117	-1	2	105	12	6				
3	91	120	-5	3	231	204	6				

ITTI LATTICE 1 (C=3.6+A) COPPER RAD. PAGE 1

-16 K 0

0	105	104	6
2	84	86	-13
4	53	55	-10

-15 K 0

1	136	123	75
3	92	84	46
5	32	30	5
7	49	35	46

-14 K 0

0	23	11	16
2	35	33	5
4	69	67	9
6	161	153	42
8	182	163	88
10	118	113	33

-13 K 0

1	47	52	-16
3	74	73	4
5	135	123	62
7	136	129	36
9	157	132	112
11	89	80	53

-12 K 0

0	198	184	65
2	214	205	42
4	123	121	10
6	34	27	15
8	29	3	29
10	-19	8	-10
12	72	69	14
14	72	77	-29

-11 K 0

1	250	248	8
3	194	186	37
5	94	92	9
7	138	131	34
9	44	35	19
11	97	89	31
13	123	111	70
15	125	115	71

-10 K 0

0	25	3	19
2	63	60	11
4	182	173	44
6	174	172	10
8	226	230	-17
10	235	224	43
12	136	130	28
14	23	18	10
16	10	2	7

-9 K 0

1	100	103	-17
3	188	185	15
5	215	216	-4
7	441	444	-8
9	198	199	-4
11	184	171	50
13	84	83	4
15	60	61	-4
17	59	55	28

-8 K 0

0	395	403	-26
2	431	431	0
4	241	243	-9
6	51	32	58
8	91	89	8
10	45	30	26
12	132	130	8
14	168	155	65
16	203	192	56
18	137	129	56

-7 K 0

1	430	434	-12
3	320	325	-19
5	190	187	15
7	257	271	-59
9	128	130	-9
11	173	164	35
13	181	186	-24
15	169	164	26
17	116	107	57

-6 K 0

0	262	248	61
2	116	113	20
4	260	266	-27
6	451	474	-65
8	462	481	-52
10	367	360	21
12	193	197	-18
14	38	18	39
16	22	21	1
18	25	17	21

-5 K 0

1	387	395	-27
3	287	299	-53
5	334	354	-76
7	206	226	-76
9	300	300	0
11	195	193	8
13	204	206	-9
15	166	163	15
17	99	95	23
19	91	87	28

-4 K 0

0	607	638	-68
2	706	751	-86
4	324	334	-39
6	212	216	-21
8	98	83	70
10	57	52	13
12	179	185	-29
14	208	203	23
16	249	241	35
18	165	157	45
20	109	106	23

-3 K 0

1	516	537	-55
3	371	391	-71
5	404	426	-72
7	64	75	-51
9	303	302	3
11	203	213	-49
13	202	203	-4
15	155	161	-31
17	112	112	0
19	102	98	27

-2 K 0

0	381	384	-10
2	57	42	75
4	410	447	-121
6	670	702	-64
8	667	687	-39
10	440	468	-85
12	214	218	-19
14	163	168	-26
16	26	15	17
18	54	52	9
20	81	78	16

-1 K 0

1	119	101	130
3	431	469	-120
5	477	472	13
7	251	271	-96
9	296	307	-45
11	239	248	-41
13	142	139	15
15	109	113	-20

TTTI LATTICE 1 (C=3.6+A) COPPER RAD. PAGE 2

17	150	145	27	4	338	353	-57		9 K	0		
19	110	112	-13	6	216	218	-10					
				8	144	139	25	1	108	105	16	
	0 K	0		10	85	82	11	3	172	170	10	
				12	180	179	4	5	199	197	9	
2	624	686	-131	14	189	186	14	7	378	377	3	
4	544	597	-133	16	194	190	19	9	208	197	46	
6	82	81	5	18	133	132	5	11	162	155	29	
8	39	0	63	20	83	90	-60	13	82	82	0	
10	115	118	-17					15	57	57	0	
12	164	165	-5		5 K	0		17	36	**	-51	
14	438	430	22									
16	227	220	30	1	401	411	-33		10 K	0		
18	194	185	45	3	267	271	-18					
20	84	85	-7	5	341	351	-37	0	26	3	21	
				7	237	248	-53	2	77	76	4	
	1 K	0		9	325	314	38	4	158	154	20	
				11	209	207	8	6	178	167	52	
1	96	67	204	13	170	176	-30	8	157	152	23	
3	431	458	-84	15	121	125	-21	10	197	175	85	
5	496	490	15	17	68	69	-5	12	107	105	9	
7	310	317	-28	19	70	70	0	14	55	54	5	
9	345	367	-80					16	35	43	-50	
11	261	269	-35		6 K	0						
13	127	130	-15						11 K	0		
15	62	72	-41	0	263	248	66					
17	111	112	-5	2	122	120	13	1	259	247	49	
19	92	92	0	4	253	258	-23	3	193	185	39	
				6	414	423	-27	5	100	96	19	
	2 K	0		8	408	408	0	7	122	121	5	
				10	326	294	102	9	57	**	33	
0	384	384	0	12	180	185	-23	11	78	74	16	
2	53	30	95	14	40	36	10	13	88	84	25	
4	422	444	-69	16	52	57	-21	15	87	86	7	
6	644	657	-27	18	48	47	5					
8	640	650	-20						12 K	0		
10	418	433	-46		7 K	0						
12	210	213	-14					0	199	184	69	
14	177	182	-25	1	458	459	-2	2	202	190	57	
16	42	35	20	3	310	313	-8	4	121	114	34	
18	67	64	16	5	186	191	-27	6	59	56	10	
20	75	74	7	7	208	216	-36	8	38	35	6	
				9	115	114	4	10	52	49	9	
	3 K	0		11	140	136	16	12	66	64	11	
				13	154	157	-14					
1	523	543	-53	15	159	155	21		13 K	0		
3	389	405	-54	17	105	104	6					
5	390	403	-43					1	61	57	15	
7	61	50	41		8 K	0		3	67	62	21	
9	242	245	-13					5	119	110	46	
11	179	186	-35	0	399	403	-12	7	124	112	59	
13	202	201	4	2	423	414	26	9	122	105	79	
15	176	172	20	4	230	227	14	11	78	75	20	
17	142	140	11	6	52	47	15					
19	105	103	13	8	45	20	44		14 K	0		
				10	84	84	0					
	4 K	0		12	122	122	0	0	20	11	11	
				14	124	117	38	2	42	39	10	
0	615	638	-50	16	128	124	25	4	73	70	15	
2	692	718	-53					6	118	108	53	

8	127	113	73		-12 K 1			-3	175	177	-9
10	70	70	0					-1	131	131	0
				-12	71	78	-34	1	136	132	18
	15 K 0			-10	70	72	-6	3	120	123	-13
				-8	45	62	-24	5	193	200	-31
1	138	122	89	-6	52	45	16	7	270	284	-54
3	90	81	51	-4	108	111	-12	9	332	341	-30
5	51	44	28	-2	186	190	-18	11	153	156	-10
7	5	3	1	0	240	249	-38	13	111	115	-17
				2	236	240	-17	15	77	84	-35
	16 K 0			4	200	207	-31	17	50	54	-24
				6	105	110	-21				
0	112	104	51	8	20	12	5		-8 K 1		
2	82	77	30	10	40	22	23				
				12	48	49	-2	-16	102	107	-28
	-16 K 1							-14	131	135	-19
					-11 K 1			-12	121	123	-7
-2	98	105	-41					-10	78	79	-2
0	132	142	-61	-13	108	112	-22	-8	57	49	16
2	139	153	-85	-11	91	94	-11	-6	106	105	3
				-9	81	79	5	-4	141	136	22
	-15 K 1			-7	87	84	7	-2	280	275	19
				-3	153	155	-9	0	443	440	8
-7	33	31	5	-1	222	228	-25	2	416	415	3
-5	43	40	8	1	282	292	-39	4	310	306	14
-3	94	102	-40	3	222	233	-47	6	159	154	22
-1	137	140	-16	5	157	166	-41	8	162	162	0
1	167	172	-26	7	119	121	-5	10	26	18	5
3	144	146	-10	9	119	117	7	12	44	40	6
5	95	101	-30	11	79	80	-3	14	145	145	0
7	34	31	6	13	95	102	-35	16	154	154	0
				15	125	130	-33				
	-14 K 1								-7 K 1		
					-10 K 1						
-8	121	124	-14					-17	78	81	-16
-6	165	171	-28	-14	50	46	14	-15	106	105	4
-4	123	131	-40	-12	87	84	11	-13	161	167	-26
-2	86	94	-36	-10	146	141	15	-11	122	121	3
0	35	40	-11	-8	232	243	-43	-9	120	109	34
2	29	24	8	-6	142	145	-13	-7	130	130	0
4	83	85	-8	-4	222	221	4	-5	200	200	0
6	130	138	-40	-2	109	107	8	-3	217	213	18
8	231	219	48	0	44	39	10	-1	269	274	-21
10	160	175	-87	2	35	13	26	1	469	450	51
				4	94	91	11	3	269	270	-4
	-13 K 1			6	239	246	-28	5	233	232	4
				8	150	166	-69	7	174	173	4
-11	75	80	-28	10	289	282	23	9	205	208	-11
-9	124	125	-4	12	165	166	-4	11	126	121	15
-7	139	143	-17	14	84	88	-19	13	125	130	-21
-5	137	147	-47	16	16	6	14	15	157	163	-30
-3	130	133	-14					17	88	91	-16
-1	74	75	-3		-9 K 1						
1	105	105	0						-6 K 1		
3	82	86	-15	-15	48	44	14				
5	133	139	-28	-13	78	75	11	-18	46	42	12
7	152	156	-18	-11	102	108	-19	-16	27	22	8
9	153	149	15	-9	177	177	0	-14	20	13	5
11	135	137	-11	-7	268	274	-22	-10	224	220	13
				-5	334	341	-24	-8	331	328	10

-6	390	391	-3	-19	34	35	-3	9	101	94	29
-4	337	329	28	-17	86	82	17	11	107	105	8
-2	120	106	71	-15	115	117	-8	13	130	135	-21
0	98	100	-10	-13	113	112	3	15	25	0	16
2	218	206	56	-11	140	142	-8	17	90	95	-22
4	129	117	60	-9	124	123	3	19	60	58	9
6	308	301	25	-7	109	104	16				
8	392	399	-21	-5	41	23	34		0 K 1		
10	399	364	90	-3	321	286	124				
12	229	225	16	-1	333	282	175	-20	36	36	0
14	66	63	8	1	366	281	258	-18	73	70	13
16	46	41	13	3	331	297	119	-14	230	225	20
18	7	9	-1	5	232	212	88	-12	281	286	-19
				7	182	171	44	-10	15	15	0
	-5 K 1			9	59	67	-20	-8	91	107	-73
				11	187	178	38	-6	108	113	-22
-19	32	36	-16	13	123	128	-21	-4	14	25	-8
-17	58	57	3	15	101	95	25	-2	478	466	31
-15	50	49	2	17	78	81	-13	0	809	776	53
-13	129	135	-25	19	49	52	-14	2	1382	1230	116
-11	135	137	-7					4	306	277	96
-9	208	201	23		-2 K 1			6	108	84	94
-7	224	224	0					8	59	58	3
-5	186	181	24	-20	68	69	-6	10	91	95	-16
-3	283	272	44	-18	21	18	4	12	51	41	22
-1	176	153	116	-16	25	4	18	14	146	143	13
1	469	430	103	-14	27	1	18	16	262	248	55
3	221	203	82	-12	127	125	8	18	108	104	21
5	257	252	21	-10	221	218	12	20	74	72	13
7	191	194	-13	-8	373	380	-22				
9	150	146	13	-6	704	634	123		1 K 1		
11	174	180	-23	-4	337	314	79				
15	162	166	-18	-2	181	131	226	-17	43	48	-13
17	84	88	-19	0	194	173	100	-15	99	98	4
19	74	75	-6	2	95	42	194	-13	63	55	20
				4	60	20	90	-11	119	115	16
	-4 K 1			6	313	283	99	-9	111	107	17
				8	568	546	50	-7	136	136	0
-18	79	82	-15	10	363	361	6	-5	159	157	9
-16	145	144	4	12	235	234	4	-3	155	151	20
-14	165	165	0	14	79	77	6	-1	293	300	-28
-12	132	124	31	16	44	40	9	1	473	477	-11
-10	102	93	29	18	14	12	2	3	199	180	89
-8	69	72	-5					5	119	110	37
-6	149	128	96		-1 K 1			7	240	238	8
-4	119	95	116					9	167	160	32
-2	447	414	91	-19	43	43	0	11	149	150	-4
0	631	555	145	-17	34	39	-11	13	124	125	-4
2	540	482	130	-15	84	89	-18	15	51	47	9
4	481	451	78	-13	61	50	27	17	30	35	-10
6	96	63	124	-11	137	138	-4	19	22	23	-2
8	133	107	90	-9	141	141	0				
10	43	55	-22	-7	211	208	13		2 K 1		
12	73	63	27	-5	180	171	38				
14	130	127	13	-3	219	181	138	-18	-15	1	-8
16	150	147	14	-1	535	406	285	-16	25	34	-15
18	159	157	11	1	524	375	314	-14	33	38	-8
				3	385	325	118	-12	89	99	-35
	-3 K 1			5	162	140	92	-10	186	186	0
				7	203	197	27	-8	348	347	3

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-6	546	574	-69					13	17	30	-15
-4	244	259	-69	-19	14	7	9	15	75	76	-4
-2	82	68	62	-17	39	36	8	17	53	49	19
0	159	179	-119	-15	15	7	5				
2	65	37	96	-13	92	100	-29		8 K	1	
4	27	21	10	-11	72	65	15				
6	217	208	38	-9	104	103	3	-16	94	90	23
8	446	429	45	-7	125	128	-14	-14	119	109	46
10	274	273	3	-5	57	62	-17	-12	65	48	40
12	177	179	-8	-3	132	137	-28	-10	32	28	4
14	57	56	2	-1	9	4	2	-8	89	81	25
16	48	48	0	1	173	192	-107	-6	250	251	-4
18	21	15	9	3	33	38	-12	-4	26	15	12
				5	93	97	-19	-2	104	113	-39
	3 K	1		7	114	113	4	0	228	230	-8
				9	91	87	10	2	166	171	-24
-19	7	6	0	11	129	124	17	4	123	130	-31
-17	51	51	0	13	48	50	-4	6	22	31	-11
-15	67	66	3	15	56	60	-12	8	137	128	34
-13	66	71	-14	17	-7	14	-10	10	63	43	31
-11	95	96	-2					12	-10	1	-2
-9	64	63	2		6 K	1		14	39	40	-2
-7	21	44	-37					16	34	34	0
-5	80	76	17	-18	13	1	9				
-3	182	185	-16	-16	62	55	25		9 K	1	
-1	195	213	-99	-14	78	75	10				
1	207	222	-78	-12	41	58	-33	-15	34	18	36
3	236	241	-23	-10	148	150	-6	-13	16	2	7
5	126	124	10	-8	244	253	-37	-11	25	9	9
7	51	53	-5	-6	275	282	-28	-9	94	93	3
9	84	65	45	-4	186	202	-82	-7	155	153	8
11	59	59	0	-2	31	23	15	-5	248	257	-37
13	68	69	-3	0	159	164	-27	-3	24	26	-2
15	68	68	0	2	269	277	-34	-1	16	18	-1
17	79	79	0	4	20	27	-10	1	53	38	34
19	49	51	-10	6	123	123	0	3	50	39	23
				8	207	209	-8	5	40	46	-12
	4 K	1		10	193	172	65	7	106	106	0
				12	91	94	-9	9	196	187	33
-18	72	70	10	14	30	21	13	11	56	51	10
-16	137	134	14	16	39	34	13	13	30	31	-2
-14	147	146	4	18	14	5	11	15	12	5	6
-12	81	70	31								
-10	28	22	5		7 K	1			10 K	1	
-8	153	164	-48								
-6	38	24	26	-17	37	33	12	-14	50	43	24
-4	20	15	6	-15	49	48	2	-12	12	5	3
-2	246	258	-56	-13	113	121	-33	-10	71	65	13
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2	294	310	-66	-9	-25	16	-16	-6	34	20	19
4	271	283	-51	-7	22	4	11	-4	64	65	-2
6	24	13	12	-5	52	69	-51	-2	39	15	32
8	54	57	-6	-3	52	52	0	0	75	63	36
10	54	50	7	-1	124	130	-31	2	85	69	51
12	16	21	-4	1	282	290	-32	4	21	13	6
14	63	63	0	3	141	144	-15	6	59	67	-22
16	82	78	16	5	81	82	-3	8	6	1	0
18	83	80	16	7	4	5	0	10	65	64	2
				9	31	29	2	12	34	40	-14
	5 K	1		11	-5	4	0	14	16	19	-7

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11 K 1

-13	80	69	55
-11	19	18	0
-9	22	9	8
-7	54	40	30
-5	24	34	-14
-3	21	10	9
-1	91	83	30
1	132	133	-4
3	87	84	11
5	31	40	-16
7	21	2	13
9	-19	16	-12
11	20	18	3
13	6	12	-7

12 K 1

-12	-10	7	-7
-10	19	17	1
-8	65	53	30
-6	84	69	51
-4	31	8	25
-2	51	51	0
0	88	84	17
2	60	56	14
4	16	8	0
6	-15	7	-7
8	38	29	15
10	24	10	19
12	8	0	4

13 K 1

-11	-8	12	-11
-9	57	48	24
-7	64	63	3
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-3	29	28	1
-1	40	30	19
1	33	9	31
3	36	19	27
5	-34	12	-44
7	36	36	0
9	35	35	0

14 K 1

-8	60	58	7
-6	96	93	13
-4	28	40	-27
-2	14	11	2
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4	15	0	9
6	15	17	-2
8	32	47	-64

15 K 1

-10	86	62	68
-8	-9	10	-7
-6	44	39	16
-4	69	62	31
-2	47	43	13
0	1	11	-3

-15 K 2

-13	24	10	19
-11	53	55	-8
-9	83	83	0
-7	85	91	-31

-14 K 2

-12	30	34	-9
-10	-13	0	-6
-8	55	59	-14
-6	23	27	-7
-4	38	30	16

-13 K 2

-11	37	37	0
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-7	64	63	2
-5	34	22	14
-3	24	8	16
-1	18	22	-4
1	19	13	5
3	67	62	15
5	51	58	-24

-12 K 2

-10	22	20	2
-8	16	15	0
-6	20	26	-7
-4	22	30	-11
-2	38	43	-10
0	123	126	-13
2	121	129	-37
4	122	127	-22
6	51	50	2
8	23	22	1
10	55	68	-47

-11 K 2

-13	41	44	-14
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-10 K 2

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8	107	120	-48
10	48	66	-36
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-9 K 2

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-3	92	96	-14
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9	197	188	32
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-8 K 2

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-4	193	195	-8
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2	226	224	8
4	210	205	21
6	40	47	-13

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				-3	-94	35	-203	6	19	7	7
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0 K -9

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4	53	24	4

0 K -8

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	6 K 11			4	89	28	9	-11	306	293	11
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	7 K 3							-9	120	125	-1
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					9 K	9		-3	37	26	9
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-10	98	157	-18	-5	-85	4	-9	-1	232	211	11
-9	99	52	9	-4	-79	1	-8	0	27	132	-20
-8	-86	14	-10	-3	92	67	5	1	83	20	8
-7	105	34	16	-2	-73	30	-9	2	97	45	9
-6	76	76	0	-1	158	144	5	3	-99	43	-14
-5	85	73	2	0	210	207	1				
-4	136	131	2	1	63	102	-8		10 K 3		
-3	172	198	-14	2	-96	30	-14				
-2	69	30	7	3	-39	24	-3	-11	51	14	3
-1	-44	9	-3	4	136	133	1	-10	125	36	20
0	-23	11	-1					-9	102	66	8
1	122	122	0		10 K -1			-8	100	35	12
2	197	205	-5					-7	158	172	-6
3	46	103	-14	-7	62	8	5	-6	227	221	3
4	32	24	0	-6	-118	35	-20	-5	112	105	2
5	83	57	5	-5	81	63	3	-4	43	84	-7
6	146	110	12	-4	174	181	-2	-3	77	79	0
7	54	49	0					-2	79	100	-4
					10 K 0			-1	299	265	21
	9 K	7						0	175	178	-1
				-10	68	70	0	1	118	39	17
-10	63	24	4	-9	96	128	-10	2	-42	61	-7
-9	-70	47	-9	-8	57	62	0	3	114	76	9
-8	58	37	2	-7	68	15	7	4	59	53	0
-7	117	121	-1	-6	101	75	6				
-6	133	117	5	-5	68	14	6		10 K 4		
-5	-51	14	-4	-4	129	115	4				
-4	-56	6	-5	-3	67	95	-6	-11	-49	103	-14
-3	102	66	9	-2	-113	15	-17	-10	96	16	11
-2	44	22	2	-1	66	73	-1	-9	81	40	6
-1	-41	101	-20	0	96	132	-10	-8	63	66	0
0	114	99	5					-7	73	0	7
1	189	206	-10		10 K 1			-6	59	68	-1
2	170	139	15					-5	-42	19	-3
3	-111	26	-21	-11	59	59	0	-4	90	16	14
4	120	47	20	-10	26	72	-6	-3	199	167	18
5	84	95	-3	-9	113	25	19	-2	208	215	-4

-1	120	109	3	4	-34	36	-3	-7	72	60	2
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1	89	42	9		10 K 7			-5	36	3	1
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3	214	202	5	-8	186	180	2	-3	129	96	9
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				-6	95	57	7	-1	106	65	8
	10 K 5			-5	60	14	4				
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-10	68	57	1	-3	197	208	-5				
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-8	221	193	13	-1	35	25	0	-7	-37	69	-6
-7	251	255	-2	0	71	82	-2	-6	154	107	15
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-5	0	59	-4	2	80	21	9	-4	118	32	19
-4	80	45	6	3	-93	5	-14	-3	-44	25	-3
-3	90	109	-6	4	-30	51	-4	-2	-101	30	-14
-2	252	259	-5					-1	49	64	-2
-1	110	107	1		10 K 8			0	40	25	1
0	96	29	14								
1	117	66	14	-5	201	154	22		11 K 5		
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				-1	-52	35	-6	-5	-27	32	-2
	10 K 6			0	148	139	3	-4	58	84	-5
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-7	61	80	-3		11 K 2			0	-44	75	-10
-6	-74	19	-8								
-5	101	14	15	-7	-73	45	-10		11 K 6		
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-3	210	212	-1	-5	113	109	1	-6	75	37	5
-2	96	89	2	-4	23	22	0	-5	0	52	-3
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0	-35	74	-10					-3	43	4	2
1	146	138	3		11 K 3			-2	21	23	0
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3	168	155	5	-8	76	25	7	0	117	143	-9