The Crystal and Molecular Structure of 2-Methyl-4-phenyl-thiothiophthene

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An X-ray structure study of crystals of 2-methyl-4-phenyl-thio-thiophthene has been carried out. The crystals belong to the monoclinic space group $P2_1/c$, with unit cell dimensions $a = 9.566$ Å, $b = 6.683$ Å, $c = 18.603$ Å, and $\beta = 94.9°$. There are four molecules per unit cell.

The structure was solved by three-dimensional Patterson synthesis, and refined by least squares methods. The refinement comprises 1931 $h0l - h6l$ reflections.

Unequal S — S distances occur in the linear three-sulphur sequence of the molecule: $S(1) - S(2) = 2.481(2)$ Å, $S(2) - S(3) = 2.242(2)$ Å, with the angle $S(1) - S(2) - S(3) = 176.5(1)°$. The other bond lengths in the thiothiophthene system are $S(1) - C(1) = 1.691(5)$ Å, $S(2) - C(3) = 1.751(4)$ Å, $S(3) - C(5) = 1.696(5)$ Å, $C(1) - C(2) = 1.387(6)$ Å, $C(2) - C(3) = 1.397(6)$ Å, $C(3) - C(4) = 1.442(5)$ Å, and $C(4) - C(5) = 1.366(6)$ Å.

The C — C bonds which connect the methyl group and the phenyl group to the thiothiophthene system, $C(1) - C(6)$ and $C(4) - C(7)$, are 1.514(8) Å, and 1.483(6) Å, respectively.

The S — S, S — C, and C — C bond lengths have been corrected for libration.

The phenyl group is planar within the error, and the thiothiophthene system is nearly so. The phenyl group is twisted 69.7° about the connection bond $C(4) - C(7)$.

In crystals of 2-methyl-4-phenyl-thiothiophthene, S(2) and S(3) of the reference molecule approaches the plane of the thiothiophthene system of a screw axis-related molecule at distances of 3.40 and 3.38 Å, respectively; the angle between the planes of the respective thiothiophthene systems is 88.5°.

The lengths of the sulphur-sulphur bonds in 2,4-diphenyl-thiothiophthene (I), 2.50 and 2.22 Å,[1] and the lengths of those in 2,5-diphenyl-thio-
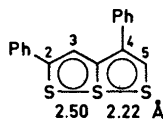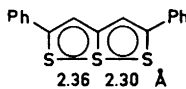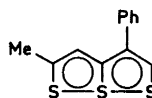
(I)   (II)   (III)

thiophthene (II), 2.36 and 2.30 Å,[2] show that the effect of phenyl substituents on the three-center bond in thiothiophthene depends on the positions of the phenyl groups. A better understanding of the bonding in the thiothiophthene system might be obtained from investigations of the relative effects of different substituents on the three-center bond. We have therefore carried out an X-ray study of 2-methyl-4-phenyl-thiothiophthene.

STRUCTURE DETERMINATION

A brief account of the structure determination has been reported earlier,[3] and a more detailed description is given here.

Crystals of 2-methyl-4-phenyl-thiothiophthene (III) were generously supplied by Klingsberg.[4] The crystals are deep red and belong to the monoclinic space group $P2_1/c$.

The structure analysis is based on photographic data, taken with Weissenberg camera and $CuK\alpha$ radiation. The data comprise 2370 $h0l - h6l$ reflections, including 433 unobserved.

Approximate coordinates for the sulphur atoms and the carbon atoms of the thiothiophthene system were found from a three-dimensional Patterson map, and the carbon atom of the methyl group and those of the phenyl group revealed themselves during a subsequent Fourier synthesis.

The structure was refined by a full-matrix least squares procedure which minimizes the function

$$r = \sum W(|F_o| - K|F_c|)^2$$

with $W = [(Ka_1)^2 + (a_2F_o)^2/4W_o]^{-1}$. W_o in the weighting scheme is an individual weight which is estimated from the assumed reliability of the intensity measurement. The constants a_1 and a_2 were in the present case set equal to 1.0. Unobserved reflections with $K|F_c|$ greater than $F_o^{\text{threshold}}$ were included in the refinement with $F_o = F_o^{\text{threshold}}$. Anisotropic temperature factors were applied to sulphur and carbon, and isotropic to hydrogen. Fifteen low order reflections, supposed to be affected by secondary extinction, were excluded from the least squares refinement. The final R factor is 7.3 % when unobserved reflections are included, and 7.1 % when they are omitted.

A rigid-body analysis of the 2-methyl-4-phenyl-thiothiophthene molecule has been carried out according to the method of Schomaker and Trueblood,[5] and the $S - S$, $S - C$, and $C - C$ bond lengths have been corrected for rigid-body libration according to Cruickshank's formula.[6] For further details with respect to the structure determination, see Experimental.

DISCUSSION

Molecular shape and dimensions. Bond lengths and angles in the 2-methyl-4-phenyl-thiothiophthene molecule, together with their standard deviations, are listed in Tables 1 and 2, and shown in Figs. 1a and 1b.

The molecule is presented in Figs. 1a and 1b in a projection on to the least squares plane of the thiothiophthene system. The equation for this plane,

Table 1. Bond lengths (l) in 2-methyl-4-phenyl-thiothiophthene. Standard deviations in parentheses. Bond length values corrected for rigid-body libration are also given. The corrections in (l') are based on the libration tensor one arrives at by treating the whole molecule as a rigid body, and the corrections in (l'') are based on the respective libration tensors one gets when the phenyl group and the thiothiophthene system are treated separately.

Bond	l'' (Å)	l' (Å)	l (Å)
S(1) – S(2)	2.481	2.480	2.475 (2)
S(2) – S(3)	2.242	2.242	2.237 (2)
S(1) – C(1)	1.691	1.691	1.688 (5)
S(2) – C(3)	1.751	1.751	1.747 (4)
S(3) – C(5)	1.696	1.696	1.693 (5)
C(1) – C(2)	1.387	1.386	1.385 (6)
C(1) – C(6)	1.514	1.514	1.510 (8)
C(2) – C(3)	1.397	1.397	1.393 (6)
C(3) – C(4)	1.442	1.441	1.439 (5)
C(4) – C(5)	1.366	1.366	1.362 (6)
C(4) – C(7)	1.483	1.483	1.480 (6)
C(7) – C(8)	1.391	1.386	1.383 (6)
C(7) – C(12)	1.399	1.393	1.389 (7)
C(8) – C(9)	1.383	1.383	1.380 (8)
C(9) – C(10)	1.375	1.369	1.365 (8)
C(10) – C(11)	1.387	1.382	1.378 (7)
C(11) – C(12)	1.396	1.395	1.393 (7)

Bond	l (Å)	Bond	l (Å)
C(2) – H(1)	0.96 (9)	C(8) – H(6)	0.99 (5)
C(5) – H(2)	0.95 (5)	C(9) – H(7)	0.90 (6)
C(6) – H(3)	0.96 (7)	C(10) – H(8)	0.89 (5)
C(6) – H(4)	0.89 (7)	C(11) – H(9)	0.87 (6)
C(6) – H(5)	1.06 (7)	C(12) – H(10)	1.03 (6)
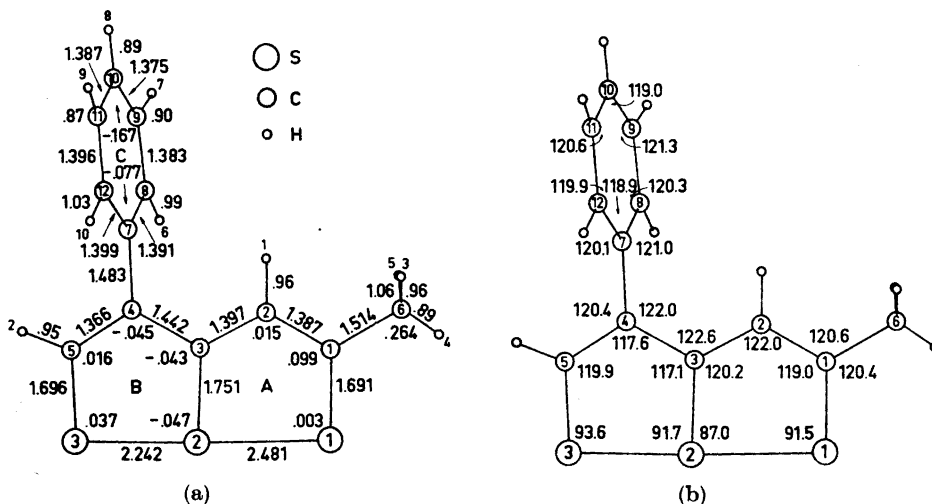
Fig. 1. (a) Bond lengths (Å) in the 2-methyl-4-phenyl-thiothiophthene molecule, and atomic distances (Å) from the least squares plane of the thiothiophthene system. (b) Bond angles (°).

Table 2. Bond angles ∠(ijk) in 2-methyl-4-phenyl-thiothiophthene. Standard deviations in parentheses refer to the last digits of respective values.

i	j	k	∠(ijk)°	i	j	k	∠(ijk)°
C(1)	S(1)	S(2)	91.5 (1)	C(10)	C(11)	C(12)	120.6 (5)
S(1)	S(2)	C(3)	87.0 (1)	C(11)	C(12)	C(7)	119.9 (4)
S(1)	S(2)	S(3)	176.5 (1)	C(1)	C(2)	H(1)	119 (8)
C(3)	S(2)	S(3)	91.7 (1)	H(4)	C(2)	C(3)	119 (7)
S(2)	S(3)	C(5)	93.6 (1)	C(4)	C(5)	H(2)	126 (3)
S(1)	C(1)	C(2)	119.0 (3)	S(3)	C(5)	H(2)	114 (3)
S(1)	C(1)	C(6)	120.4 (4)	C(1)	C(6)	H(3)	113 (4)
C(6)	C(1)	C(2)	120.6 (5)	C(1)	C(6)	H(4)	114 (4)
C(1)	C(2)	C(3)	122.0 (4)	C(1)	C(6)	H(5)	99 (4)
C(2)	C(3)	C(4)	122.6 (4)	H(3)	C(6)	H(4)	121 (6)
C(2)	C(3)	S(2)	120.2 (3)	H(3)	C(6)	H(5)	106 (6)
S(2)	C(3)	C(4)	117.1 (3)	H(4)	C(6)	H(5)	99 (6)
C(3)	C(4)	C(7)	122.0 (3)	C(7)	C(8)	H(6)	116 (2)
C(3)	C(4)	C(5)	117.6 (4)	H(6)	C(8)	C(9)	123 (2)
C(5)	C(4)	C(7)	120.4 (3)	C(8)	C(9)	H(7)	117 (4)
C(4)	C(5)	S(3)	119.9 (3)	H(7)	C(9)	C(10)	121 (4)
C(4)	C(7)	C(8)	121.0 (4)	C(9)	C(10)	H(8)	128 (3)
C(4)	C(7)	C(12)	120.1 (4)	H(8)	C(10)	C(11)	113 (3)
C(8)	C(7)	C(12)	118.9 (4)	C(10)	C(11)	H(9)	114 (4)
C(7)	C(8)	C(9)	120.3 (5)	H(9)	C(11)	C(12)	124 (4)
C(8)	C(9)	C(10)	121.3 (5)	C(11)	C(12)	H(10)	123 (3)
C(9)	C(10)	C(11)	119.0 (5)	H(10)	C(12)	C(7)	117 (3)

with weights inversely proportional to standard deviations in atomic co-ordinates, is

$$0.48310\,X + 0.71670\,Y - 0.54259\,Z = 0.28563$$

with X, Y, and Z in Å units. Deviations from the plane for the atoms of the thiothiophthene system, the atom C(6) of the methyl group, and the atoms C(7) and C(10) of the phenyl group, are given in Fig. 1a. It is seen that the thiothiophthene system is nearly planar. The methyl group and the phenyl group point slightly out of the plane.

The equation for the least squares plane through the carbon atoms of the phenyl group is

$$0.57543\,X - 0.30343\,Y + 0.70725\,Z = 5.96468$$

and the deviations in Å units from this plane are C(7) −0.002, C(8) −0.004, C(9) 0.009, C(10) −0.006, C(11) 0.000, and C(12) 0.005.

The twist angle of the phenyl group about C(4)−C(7) is 69.7°. The twist angle was taken as the angle between the plane through C(3), C(4), C(5), and C(7), and the plane through C(4), C(7), C(8), and C(12).

Comparison with the structure of 2,4-diphenyl-thiothiophthene. Bond lengths in 2,4-diphenyl-thiothiophthene [1] are given in Fig. 2. The bond lengths include correction for rigid-body libration. The rigid-body analysis has been carried out according to the method of Schomaker and Trueblood,[5] and the bond lengths are corrected according to Cruickshank's formula.[6]
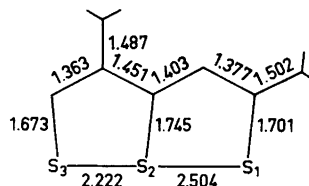
Fig. 2. Bond lengths (Å) in 2,4-diphenyl-
thiothiophthene.

The sulphur-sulphur bond lengths in 2-methyl-4-phenyl-thiothiophthene (*cf.* Fig. 1a) are S(1) − S(2) = 2.481(2) Å, and S(2) − S(3) = 2.242(2) Å. In 2,4-diphenyl-thiothiophthene, the equivalent bonds are 2.504(3) and 2.222(3) Å, respectively (*cf.* Fig. 2). From these bond lengths, the exchange of the 2-phenyl group in the latter compound with a methyl group leaves the bonding in the sulphur sequence almost unchanged.

There is close agreement between the C − C bond lengths in the thio-thiophthene system of the 2-methyl-4-phenyl derivative and those in the 2,4-diphenyl derivative; they are 1.387(6), 1.397(6), 1.442(5), and 1.366(6) Å in the former, and 1.377(11), 1.403(9), 1.451(11), and 1.363(9) Å in the latter, reckoned in the same order. Also, the carbon-sulphur bond lengths in the two derivatives agree, being 1.691(5), 1.751(4), and 1.696(5)Å in the former, and 1.701(5), 1.745(5), and 1.673(7) Å in the latter.

The crystal structure. The arrangement of the 2-methyl-4-phenyl-thio-thiophthene molecules in the unit cell, as seen along the *b*-axis, is shown in Fig. 3. One should note the way in which the molecule in position (T) is arranged relative to the reference molecule (*R*). Molecule (*T*) lies *b*/2 above (*R*). and the plane of the thiothiophthene system in (*T*) and that of the thio-thiophthene system in (*R*) are nearly perpendicular to each other; the angle
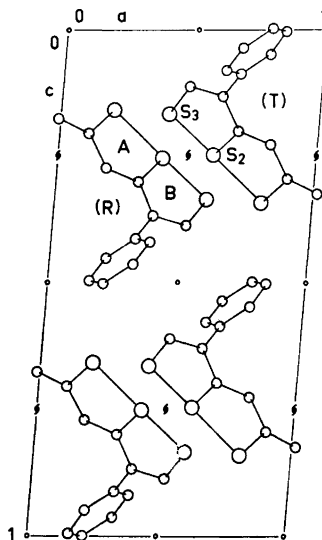
Fig. 3. The arrangement of 2-methyl-4-phenyl-thiothiophthene molecules as seen along the *b*-axis.

Table 3. Intermolecular atomic distance $D(ij)$ showing the way in which S(2) and S(3) of the molecule in position (T) approach the atoms of rings A and B of the molecule in position (R).

i	j	$D(ij)$	i	j	$D(ij)$
S(2)	S(2)$_B$	3.864 (3)	S(3)	S(1)$_A$	3.911 (3)
S(2)	S(3)$_B$	3.694 (3)	S(3)	S(2)$_A$	3.792 (3)
S(2)	C(3)$_B$	3.686 (5)	S(3)	C(1)$_A$	3.617 (5)
S(2)	C(4)$_B$	3.598 (5)	S(3)	C(2)$_A$	3.518 (5)
S(2)	C(5)$_B$	3.533 (5)	S(3)	C(3)$_A$	3.539 (5)

between the planes is 88.5°. The distances at which S(2) and S(3) of molecule (T) approach the atoms of rings B and A of molecule (R) are given in Table 3. It is seen that the sulphur atoms are located almost exactly above the centers of the respective rings.

The distance from S(3) in molecule (T) to the plane of ring A in molecule (R), and the distance from S(2) in (T) to the plane of ring B in (R) are 3.38 and 3.40 Å, respectively. These distances are shorter than the sum, 3.55 Å,[7] of the van der Waals radius for sulphur and the half-thickness of an aromatic molecule. A similar close contact of 3.25 Å occurs in the crystals of 2,5-diphenyl-thiothiophthene,[2] and that contact may, at least in part, explain why the sulphur-sulphur bonds there are of different lengths. If, in the present structure, the close contacts in which S(2) and S(3) are involved are established through a transfer of negative charge towards these atoms, S(3) might become less electronegative than S(1). This would (*cf.* the bonding in the linear trihalide ions [8-11] lengthen the S(1) − S(2) bond, and shorten the S(2) − S(3) bond. It is likely, therefore, that the difference between the sulphur-sulphur bonds in 2,4-diphenyl-thiothiophthene, and the sulphur-sulphur bonds in an *isolated* 2-methyl-4-phenyl-thiothiophthene molecule would be somewhat greater than indicated by the S − S bond lengths above.

EXPERIMENTAL

The unit cell dimensions for crystals of 2-methyl-4-phenyl-thiothiophthene were determined from high-order reflections on $h0l$ and $0kl$ Weissenberg photographs, where sodium chloride powder lines had been superimposed for reference ($a_{NaCl} = 5.6394$ Å). A least squares procedure on 52 measured 2θ-values gave $a = 9.566(2)$ Å, $b = 6.683(2)$ Å, $c = 18.603(3)$ Å, and $\beta = 94.93(2)°$.

Four formula units per unit cell give a calculated density of 1.404 g/cm³, as compared with the density, 1.404 g/cm³, found by flotation.

The intensities of the $h0l − h6l$ and $0kl$ reflections were estimated visually from Weissenberg photographs taken with Ni-filtered Cu$K\alpha$ radiation ($\mu = 51.74$ cm⁻¹). $0kl$ reflections from the zero layer about a were used for scaling only.

Lp corrections and absorption corrections were applied, the latter according to a procedure of Coppens, Leiserowitz and Rabinovich.[12] The dimension of the intensity crystal was 0.25 mm in each of the three axial directions. A grid of $8 \times 8 \times 8$ points was used.

The scattering factors used for sulphur, carbon, and hydrogen in the structure factor calculations were those given in the *International Tables*.[13]

Final atomic coordinates from the least squares refinement are listed in Table 4, and the temperature parameters are listed in Table 5. A pictorial representation of the thermal motion of the S and C atoms is given in Fig. 4.

Table 4. Atomic coordinates in fractions of corresponding cell edges. Standard deviations in parentheses refer to the last digits of respective values.

Atom	x	y	z
S(1)	0.19703 (14)	0.21199 (22)	0.16224 (6)
S(2)	0.39961 (12)	0.20019 (19)	0.25431 (6)
S(3)	0.58623 (12)	0.20842 (21)	0.33539 (6)
C(1)	0.12229 (45)	0.39702 (77)	0.20639 (22)
C(2)	0.18480 (44)	0.45866 (72)	0.27258 (21)
C(3)	0.31343 (41)	0.38291 (70)	0.30114 (19)
C(4)	0.38375 (40)	0.45462 (69)	0.36769 (19)
C(5)	0.51472 (42)	0.38254 (76)	0.38721 (21)
C(6)	− 0.01167 (56)	0.49367 (103)	0.17457 (28)
C(7)	0.31947 (38)	0.60546 (68)	0.41293 (19)
C(8)	0.20762 (46)	0.55647 (78)	0.45194 (25)
C(9)	0.15382 (49)	0.69569 (89)	0.49693 (27)
C(10)	0.20681 (40)	0.88518 (81)	0.50288 (23)
C(11)	0.31860 (50)	0.93590 (80)	0.46450 (26)
C(12)	ʋ.37549 (46)	0.79696 (77)	0.41941 (23)
H(1)	− 0.004 (6)	0.636 (11)	0.1706 (34)
H(2)	− 0.058 (7)	0.421 (11)	0.1404 (37)
H(3)	− 0.076 (7)	0.466 (11)	0.2171 (37)
H(4)	0.142 (7)	0.565 (10)	0.2981 (21)
H(5)	0.576 (5)	0.427 (8)	0.4271 (26)
H(6)	0.175 (4)	0.416 (7)	0.4486 (21)
H(7)	0.078 (6)	0.661 (10)	0.5188 (32)
H(8)	0.179 (4)	0.987 (7)	0.5295 (23)
H(9)	0.339 (5)	1.063 (9)	0.4657 (28)
H(10)	0.461 (6)	0.828 (9)	0.3909 (30)

Table 5. Temperature parameters U_{ij} (Å^2) for sulphur and carbon, and U (Å^2) for hydrogen. The expressions used are $\exp[-2\pi^2(h^2a^{*2}U_{11} + \cdots 2hka^*b^*U_{12} + \cdots)]$ for sulphur and carbon, and $\exp[-8\pi^2 U(\sin^2\theta/\lambda^2)]$ for hydrogen. All values multiplied by 10^4. Standard deviations in parentheses refer to the last digits of the respective values.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
S(1)	621 (1)	527 (1)	349 (1)	42 (4)	− 137 (1)	3 (1)
S(2)	526 (2)	385 (1)	378 (1)	66 (1)	− 57 (1)	93 (1)
S(3)	452 (5)	511 (2)	462 (1)	149 (1)	− 1 (1)	34 (2)
C(1)	470 (25)	481 (37)	363 (23)	− 67 (25)	− 2 (23)	− 14 (19)
C(2)	454 (25)	360 (32)	346 (22)	− 25 (23)	− 69 (21)	16 (19)
C(3)	407 (23)	352 (31)	297 (20)	− 36 (21)	− 13 (19)	59 (17)
C(4)	386 (23)	363 (31)	311 (21)	− 47 (21)	39 (20)	33 (17)
C(5)	396 (23)	468 (36)	354 (23)	28 (24)	− 10 (22)	10 (18)
C(6)	593 (38)	936 (68)	505 (35)	184 (40)	− 190 (40)	111 (30)
C(7)	359 (21)	362 (32)	279 (19)	− 21 (20)	4 (18)	12 (16)
C(8)	424 (26)	455 (39)	558 (30)	− 133 (26)	− 132 (27)	156 (22)
C(9)	435 (27)	671 (46)	531 (30)	− 31 (30)	− 143 (30)	161 (23)
C(10)	457 (21)	562 (42)	406 (26)	104 (25)	− 168 (26)	9 (18)
C(11)	517 (33)	390 (33)	534 (33)	− 28 (30)	− 126 (31)	25 (24)
C(12)	477 (26)	411 (35)	422 (25)	− 56 (25)	− 10 (23)	55 (21)

		U			U
	H(1)	923		H(6)	121
	H(2)	702		H(7)	589
	H(3)	801		H(8)	211
	H(4)	183		H(9)	313
	H(5)	324		H(10)	500
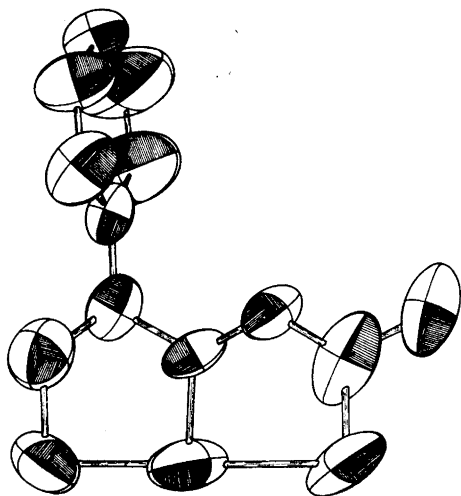
Fig. 4. Thermal ellipsoides as seen perpendicular to the plane of the thiothiophthene system.

Table 6. Results from the rigid-body analysis of the 2-methyl-4-phenyl-thiothiophthene molecule.

	Eigenvalues		Eigenvectors Direction cosines × 10^4 relative to a, b, and c^*, respectively		
Librational tensor, **L**	$\begin{cases} 14.9\ (°)^2 \\ 5.1 \\ 2.2 \end{cases}$		$\begin{matrix} -8636 \\ -620 \\ -5004 \end{matrix}$	$\begin{matrix} 4008 \\ 5174 \\ -7560 \end{matrix}$	$\begin{matrix} 3059 \\ -8335 \\ -4230 \end{matrix}$
Translational tensor, **T**	$\begin{cases} 0.0409\ Å^2 \\ 0.0341 \\ 0.0298 \end{cases}$		$\begin{matrix} -8409 \\ 1789 \\ 5107 \end{matrix}$	$\begin{matrix} 4342 \\ -3404 \\ 8341 \end{matrix}$	$\begin{matrix} 3231 \\ 9231 \\ 2085 \end{matrix}$
Symmetrized screw tensor **S**	$\begin{pmatrix} 40 \\ \\ \end{pmatrix}$	$\begin{matrix} -66 \\ 66 \\ \end{matrix}$	$\left.\begin{matrix} 56 \\ -37 \\ -107 \end{matrix}\right)$ × 10^5 rad Å		

Center of gravity of the molecule is at $x=0.33275$, $y=0.44348$, $z=0.35084$.
The origin which symmetrizes **S** is at $x=0.34896$, $y=0.49205$, $z=0.36000$.

Table 7. Librational tensors from the rigid-body analysis of certain parts of the 2-methyl-4-phenyl-thiothiophthene molecule. $\mathbf{L}_{(A+B)}$ refer to the thiothiophthene system plus C(7) and C(6). $\mathbf{L}_C$ refer to the phenyl ring plus C(4).

	Eigenvalues		Eigenvectors Direction cosines × 10^4 relative to a, b, and c^*, respectively		
$\mathbf{L}_{(A+B)}$	$\begin{cases} 14.9\ (°)^2 \\ 7.3 \\ 3.2 \end{cases}$		$\begin{matrix} -1556 \\ -8499 \\ -5034 \end{matrix}$	$\begin{matrix} 3688 \\ 4228 \\ -8278 \end{matrix}$	$\begin{matrix} 9164 \\ 3145 \\ 2477 \end{matrix}$
$\mathbf{L}_C$	$\begin{cases} 47.0\ (°)^2 \\ 8.8 \\ 3.6 \end{cases}$		$\begin{matrix} -5610 \\ -5434 \\ 6245 \end{matrix}$	$\begin{matrix} 6056 \\ 2449 \\ -7571 \end{matrix}$	$\begin{matrix} 5644 \\ -8030 \\ 1916 \end{matrix}$

Table 8. Observed and calculated structure factors for 2-methyl-4-phenyl-thiothiophthene. The values given are ten times the absolute values. Unobserved reflections are marked with a minus sign in front of F_0.

H	K	L	F(O)	F(C)
2	0	0	476	-443
3	0	0	220	-218
4	0	0	608	-609
5	0	0	864	547
6	0	0	63	37
7	0	0	34	28
8	0	0	161	-159
9	0	0	80	-77
10	0	0	326	336
11	0	0	151	-149
12	0	0	11	19
0	0	4	228	201
0	0	6	516	540
0	0	8	90	92
0	0	10	378	-365
0	0	12	616	653
0	0	14	207	-156
0	0	16	56	-56
0	0	18	118	108
0	0	20	105	52
0	0	22	140	-136
1	0	2	370	336
1	0	10	725	659
1	0	12	243	-228
1	0	14	-20	11
1	0	16	54	33
1	0	18	226	230
1	0	20	275	-317
1	0	22	141	148
1	0	-2	285	267
1	0	-4	493	-586
1	0	-6	133	120
1	0	-8	310	255
1	0	-10	86	-51
1	0	-12	234	-229
1	0	-14	430	465
1	0	-16	156	-154
1	0	-18	23	29
1	0	-20	240	261
1	0	-22	28	33
2	0	4	514	-548
2	0	6	288	-256
2	0	8	382	371
2	0	12	159	-138
2	0	12	-19	7
2	0	14	171	-169
2	0	16	-21	-29
2	0	18	52	-27
2	0	20	74	68
2	0	22	55	-55
2	0	-2	142	-50
2	0	-4	242	-246
2	0	-6	116	-124
2	0	-8	92	-67
2	0	-10	99	92
2	0	-12	-19	17
2	0	-14	168	-184
2	0	-16	287	255
2	0	-18	51	-39
2	0	-20	101	-184
2	0	-22	31	-34
3	0	2	233	-237
3	0	4	35	39
3	0	6	594	-619
3	0	8	259	-264
3	0	10	121	109
3	0	12	122	-123
3	0	14	70	-65
3	0	16	117	117
3	0	18	158	-177
3	0	20	131	-118
3	0	22	64	54
3	0	-2	48	42
3	0	-4	234	-242
3	0	-6	185	-165
3	0	-8	57	-53
3	0	-10	157	-156
3	0	-12	65	61
3	0	-14	148	-159
3	0	-16	36	35
3	0	-18	415	-469
3	0	-20	80	87
3	0	-22	-14	-24
4	0	4	670	-662
4	0	6	148	140
4	0	8	282	277
4	0	10	240	-243
4	0	12	55	-39
4	0	14	200	209
4	0	16	93	-52
4	0	18	-19	17
4	0	20	103	56
4	0	-2	401	-354
4	0	-4	151	154
4	0	-6	312	306
4	0	-8	607	-640
4	0	-10	590	554
4	0	-12	327	-347
4	0	-14	232	-247
4	0	-16	62	-58
4	0	-18	301	311
4	0	-20	201	-206
4	0	-22	128	150
5	0	2	678	-683
5	0	4	41	-26
5	0	6	334	329
5	0	8	140	122
5	0	10	519	-513
5	0	12	503	532
5	0	14	190	-189
5	0	16	-20	2
5	0	18	136	130
5	0	20	13	8
5	0	-2	176	-175
5	0	-4	153	131
5	0	-6	303	279
5	0	-8	209	183
5	0	-10	645	-638
5	0	-12	597	601
5	0	-14	63	-54
5	0	-16	41	38
5	0	-18	176	156
5	0	-20	-16	7
5	0	-22	88	-83
6	0	2	275	277
6	0	4	131	111
6	0	6	92	79
6	0	8	328	-324
6	0	10	412	412
6	0	12	212	-197
6	0	14	78	-65
6	0	16	35	-42
6	0	18	101	57
6	0	-2	309	317
6	0	-4	211	-196
6	0	-6	-19	6
6	0	-8	148	136
6	0	-10	132	128
6	0	-12	113	-107
6	0	-14	244	251
6	0	-16	69	-63
6	0	-18	27	-36
6	0	-20	66	68
7	0	2	140	-132
7	0	4	32	34
7	0	6	267	263
7	0	8	89	-87
7	0	10	49	-46
7	0	12	132	121
7	0	14	63	-54
7	0	16	39	30
7	0	18	75	-82
7	0	-2	220	-239
7	0	-4	144	140
7	0	-6	139	-135
7	0	-8	-21	-9
7	0	-10	64	62
7	0	-12	-22	16
7	0	-14	-21	-14
7	0	-16	-19	-13
7	0	-18	71	62
7	0	-20	-11	0
8	0	2	64	-58
8	0	4	30	-3
8	0	6	205	-191
8	0	8	-21	14
8	0	10	144	152
8	0	12	108	-91
8	0	14	-15	-15
8	0	16	94	110
8	0	-4	45	27
8	0	-6	159	-147
8	0	-8	246	248
8	0	-10	83	-69
8	0	-12	68	-66
8	0	-14	19	9
8	0	-16	105	110
8	0	-18	143	-158
9	0	2	229	223
9	0	6	192	-191
9	0	6	-20	2
9	0	8	81	76
9	0	10	90	-93
9	0	12	68	-62
9	0	14	124	134
9	0	-2	35	-32
9	0	-4	131	130
9	0	-6	219	215
9	0	-8	426	-434
9	0	-10	286	278
9	0	-12	81	-72
9	0	-14	121	-101
9	0	-16	71	-60
10	0	2	184	-186
10	0	4	95	77
10	0	6	59	54
10	0	8	-16	-7
10	0	10	110	-99
10	0	12	118	161
10	0	-2	128	-125
10	0	-4	92	-90
10	0	-6	-19	0
10	0	-8	50	44
10	0	-10	165	-172
10	0	-12	50	43
10	0	-14	46	-50
11	0	2	49	52
11	0	4	-14	-3
11	0	6	-13	14
11	0	-2	23	34
11	0	-4	61	-56
11	0	-6	27	-22
11	0	-8	25	-13
12	0	2	65	-66
12	0	-2	-11	-2
12	0	-4	23	-12
12	0	-6	36	-43
1	1	0	144	-136
2	1	0	318	-331
3	1	0	291	278
4	1	0	103	105
5	1	0	115	100
6	1	0	226	-208
7	1	0	-21	14
9	1	0	44	45
9	1	0	50	54
10	1	0	71	60
11	1	0	100	-94
12	1	0	13	-19
0	1	3	116	-113
0	1	3	189	-183
0	1	4	367	-391
0	1	5	423	-444
0	1	6	65	-49
0	1	7	153	-145
0	1	8	18	-24
0	1	9	145	169
0	1	10	216	196
0	1	11	142	-129
0	1	12	-20	-2
0	1	13	21	-33
0	1	14	65	-39
0	1	15	58	59
0	1	16	147	-143
0	1	17	-22	-4
0	1	18	121	134
0	1	19	-21	-8
0	1	20	30	-32
0	1	21	25	20
0	1	22	79	75
0	1	23	-12	14
1	1	1	248	253
1	1	2	439	464
1	1	3	382	397
1	1	4	623	681
1	1	5	170	165
1	1	6	84	76
1	1	7	52	-40
1	1	8	352	-347
1	1	9	289	-277
1	1	10	377	382
1	1	11	55	48
1	1	12	47	40
1	1	13	40	-42
1	1	14	28	-32
1	1	15	65	-60
1	1	16	173	184
1	1	17	-22	30
1	1	18	41	35
1	1	19	-21	-8
1	1	20	171	-169
1	1	21	-17	-11
1	1	22	112	119
1	1	23	19	24
1	1	-3	360	409
1	1	-5	35	33
1	1	-6	50	43
1	1	-7	-25	-25
1	1	-8	244	240
1	1	-9	25	22
1	1	-10	254	258
1	1	-11	215	-217
1	1	-12	101	-95
1	1	-13	312	299
1	1	-14	300	292
1	1	-15	209	-198
1	1	-16	187	-195
1	1	-17	-22	18
1	1	-18	38	42
1	1	-19	-21	18
1	1	-20	28	29
1	1	-21	32	32
1	1	-22	137	146
1	1	-23	65	-69
2	1	1	69	-46
2	1	2	622	657
2	1	3	244	261
2	1	4	692	720
2	1	5	400	418
2	1	6	596	-634
2	1	7	164	146
2	1	8	931	949
2	1	9	318	323
2	1	10	181	-167
2	1	11	30	29
2	1	12	206	-200
2	1	13	96	-98
2	1	14	144	163
2	1	15	49	47
2	1	16	197	205
2	1	17	-22	-20
2	1	18	244	-256
2	1	19	-20	-18
2	1	20	232	229
2	1	21	28	35
2	1	22	-13	-13
2	1	-1	181	-180
2	1	-6	356	-381
2	1	-7	267	275
2	1	-8	295	300
2	1	-9	109	114
2	1	-10	231	232
2	1	-11	74	-71
2	1	-12	45	-38
2	1	-13	74	-75
2	1	-14	330	-342
2	1	-15	157	147
2	1	-16	527	582
2	1	-17	-22	-3
2	1	-18	168	-174
2	1	-19	30	36
2	1	-20	62	60
2	1	-21	32	-36
2	1	-22	73	77
2	1	-23	-12	-16
3	1	1	253	-260
3	1	2	265	276
3	1	3	63	53
3	1	5	443	-457
3	1	6	772	755
3	1	7	145	140
3	1	8	156	-131
3	1	9	144	144
3	1	10	123	-105
3	1	11	137	128
3	1	12	76	72
3	1	13	51	-46
3	1	14	146	134
3	1	15	241	257
3	1	16	312	-311
3	1	17	159	-162
3	1	18	171	166
3	1	19	27	29
3	1	20	-17	-16
3	1	21	20	25
3	1	22	25	-22
3	1	-1	208	-199
3	1	-2	87	-99
3	1	-3	38	-42
3	1	-4	190	-188
3	1	-6	653	638
3	1	-7	174	-166
3	1	-8	719	-766
3	1	-9	163	160
3	1	-10	112	115
3	1	-11	93	84
3	1	-12	224	232
3	1	-13	61	59
3	1	-14	-22	24
3	1	-15	135	134
3	1	-16	228	-234
3	1	-17	86	-83
3	1	-18	292	304
3	1	-19	59	-59
3	1	-20	203	-211
3	1	-21	52	56
3	1	-22	39	-48
3	1	-23	19	27
4	1	1	32	-24
4	1	2	309	-334
4	1	3	19	-22
4	1	4	296	297
4	1	5	152	-148
4	1	6	251	-229
4	1	7	352	-343
4	1	8	160	-148
4	1	9	175	-153
4	1	10	173	-170
4	1	11	84	-70
4	1	12	249	228
4	1	13	26	22
4	1	14	212	-206
4	1	15	59	-46
4	1	16	85	80
4	1	17	38	38
4	1	18	81	-82
4	1	19	-17	-4
4	1	20	-15	3
4	1	21	24	26
4	1	-1	19	20
4	1	-2	174	-170
4	1	-3	70	62
4	1	-4	262	-252
4	1	-5	137	118
4	1	-6	343	-320
4	1	-8	418	384
4	1	-9	209	197
4	1	-10	360	-332
4	1	-11	36	-32
4	1	-12	-22	2
4	1	-13	109	-105
4	1	-14	-23	22
4	1	-15	88	-89
4	1	-16	201	-199
4	1	-17	98	-101
4	1	-18	84	-74
4	1	-19	101	100
4	1	-20	-10	8
4	1	-21	79	-75
5	1	1	179	-152
5	1	2	263	-247
5	1	3	103	102
5	1	4	164	-155
5	1	5	49	41
5	1	6	211	194
5	1	7	-18	-88
5	1	8	84	-84
5	1	9	36	30
5	1	10	-23	4
5	1	11	315	-299
5	1	12	63	-58
5	1	13	-23	6
5	1	14	32	20
5	1	15	-22	-6
5	1	16	43	-52
5	1	17	65	-60
5	1	18	111	106
5	1	19	-15	1
5	1	20	52	-54
5	1	-1	166	147
5	1	-2	235	-208
5	1	-3	38	31
5	1	-4	54	-50
5	1	-5	-18	-11
5	1	-6	65	49
5	1	-7	142	-133
5	1	-8	73	-36
5	1	-9	139	-127
5	1	-10	192	-165
5	1	-11	179	-169
5	1	-12	-23	13
5	1	-13	105	-105
5	1	-14	154	-154
5	1	-15	-23	19
5	1	-16	-22	40
5	1	-17	-22	10
5	1	-18	-20	-24
5	1	-19	77	65
5	1	-20	71	65
5	1	-21	-14	-21
5	1	-22	52	-65
6	1	1	34	-33
6	1	2	84	-81
6	1	3	-20	18
6	1	4	219	209
6	1	5	65	45
6	1	6	25	-28
6	1	7	91	-92
6	1	8	351	-351
6	1	9	219	215
6	1	10	343	349
6	1	11	85	82
6	1	12	77	-71
6	1	13	-22	-4
6	1	14	94	-99
6	1	15	54	-56
6	1	16	130	116
6	1	17	-16	-3
6	1	18	-14	-20
6	1	19	52	49
6	1	-1	166	154

Table 8. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
6	1	-4	465	452	9	1	14	45	-37	1	2	4	214	-192	3	2	-5	401	381	6	2	7	77	-60
6	1	-3	302	-251	9	1	-1	-22	12	1	2	5	132	-126	3	2	-7	401	-403	6	2	8	187	181
6	1	-4	176	-172	9	1	-2	-22	-2	1	2	6	88	-80	3	2	-8	243	-238	6	2	9	38	33
6	1	-5	-20	-22	9	1	-3	75	71	1	2	7	274	-261	3	2	-9	222	208	6	2	10	178	-178
6	1	-6	-21	-20	9	1	-4	31	29	1	2	8	434	408	3	2	-10	81	69	6	2	11	113	-108
6	1	-7	58	-52	9	1	-5	34	-42	1	2	9	215	220	3	2	-11	25	19	6	2	12	101	85
6	1	-8	64	58	9	1	-6	87	-91	1	2	10	314	-319	3	2	-12	36	36	6	2	13	32	-33
6	1	-9	74	-70	9	1	-7	64	-60	1	2	11	254	-261	3	2	-13	31	24	6	2	14	72	-80
6	1	-10	67	66	9	1	-8	87	92	1	2	12	185	181	3	2	-14	44	39	6	2	15	93	-95
6	1	-11	-23	-20	9	1	-9	92	-101	1	2	13	79	71	3	2	-15	18	14	6	2	16	59	-59
6	1	-12	257	-259	9	1	-10	-21	17	1	2	14	-15	-9	3	2	-16	91	-80	6	2	17	19	-12
6	1	-13	151	179	9	1	-11	-20	19	1	2	15	53	47	3	2	-17	54	50	6	2	18	19	-22
6	1	-14	347	366	9	1	-12	-19	2	1	2	16	107	-106	3	2	-18	85	77	6	2	19	23	-26
6	1	-15	-23	2	9	1	-13	-18	10	1	2	17	-15	-19	3	2	-19	-13	-5	6	2	-1	354	-352
6	1	-16	110	-109	9	1	-14	-17	10	1	2	18	96	-99	3	2	-20	65	-65	6	2	-2	449	-468
6	1	-17	51	57	9	1	-15	21	-24	1	2	19	82	-91	3	2	-21	27	39	6	2	-3	240	225
6	1	-18	-15	-11	9	1	-16	20	2	1	2	20	119	114	3	2	-22	33	40	6	2	-4	278	275
6	1	-19	-17	-7	9	1	-17	37	-44	1	2	21	86	88	4	2	1	188	205	6	2	-5	54	-48
6	1	-20	-14	3	10	1	1	55	55	1	2	22	114	-119	4	2	2	502	-494	6	2	-6	39	-30
6	1	-21	41	59	10	1	2	-20	-8	1	2	-5	413	-447	4	2	3	287	-298	6	2	-7	77	-68
7	1	1	63	-59	10	1	3	-20	-16	1	2	-6	190	-180	4	2	4	544	549	6	2	-8	200	-193
7	1	2	232	232	10	1	4	59	-63	1	2	-7	234	-225	4	2	5	48	41	6	2	-9	171	-170
7	1	3	73	68	10	1	5	39	-45	1	2	-8	497	-512	4	2	6	-13	3	6	2	-10	173	-168
7	1	4	67	60	10	1	6	87	82	1	2	-9	87	82	4	2	7	13	-7	6	2	-11	62	-73
7	1	5	163	162	10	1	7	-17	-27	1	2	-10	109	-109	4	2	8	264	-257	6	2	-12	209	212
7	1	6	299	-302	10	1	8	25	-36	1	2	-11	162	158	4	2	9	15	-3	6	2	-13	188	-160
7	1	7	119	-116	10	1	9	42	-60	1	2	-12	398	415	4	2	10	73	72	6	2	-14	-194	-203
7	1	8	371	407	10	1	10	32	-31	1	2	-13	179	-168	4	2	11	53	48	6	2	-15	67	63
7	1	9	40	42	10	1	11	27	-29	1	2	-14	344	-346	4	2	12	367	390	6	2	-16	59	53
7	1	10	147	-153	10	1	-1	20	-22	1	2	-15	42	43	4	2	13	322	351	6	2	-17	-13	1
7	1	11	-22	-2	10	1	-2	37	-36	1	2	-16	187	182	4	2	14	286	-304	6	2	-18	17	17
7	1	12	105	-118	10	1	-3	52	-54	1	2	-17	43	-39	4	2	15	219	-211	6	2	-19	22	-27
7	1	13	62	55	10	1	-4	-20	-5	1	2	-18	91	91	4	2	16	162	161	6	2	-20	67	-70
7	1	14	85	66	10	1	-5	28	-34	1	2	-19	-14	0	4	2	17	-14	21	7	2	1	21	-21
7	1	15	57	56	10	1	-6	66	68	1	2	-20	80	-80	4	2	18	72	64	7	2	2	33	32
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1	4	7	105	94
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1	4	11	311	323
1	4	12	51	-45
1	4	13	61	-57
1	4	14	121	-106
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1	4	16	-24	-20
1	4	17	84	-73
1	4	18	130	111
1	4	19	152	143
1	4	20	61	-49
1	4	-1	297	383
1	4	-2	248	269
1	4	-3	367	-438
1	4	-4	224	-240
1	4	-5	-20	-10
1	4	-6	51	-45
1	4	-7	45	-32

Table 8. Continued.

h	k	l	F(O)	F(C)	h	k	l	F(U)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
1	4	-8	106	95	4	4	13	47	-30	7	4	11	66	-58	0	5	10	-21	-3	3	5	-5	223	236
1	4	-9	100	-87	4	4	14	109	95	7	4	12	42	43	0	5	11	40	-27	3	5	-6	172	181
1	4	-10	66	-74	4	4	15	208	202	7	4	13	42	45	0	5	12	45	-43	3	5	-7	294	-296
1	4	-11	37	-20	4	4	16	130	-103	7	4	-1	-14	-21	0	5	13	-20	-7	3	5	-9	139	139
1	4	-12	74	-73	4	4	17	36	-30	7	4	-1	94	-90	0	5	14	-20	3	3	5	-10	44	35
1	4	-13	178	183	4	4	18	51	-47	7	4	-2	53	55	0	5	15	88	71	3	5	-11	112	-111
1	4	-14	77	77	4	4	19	40	-52	7	4	-3	51	-49	0	5	16	-17	6	3	5	-12	129	109
1	4	-15	245	-241	4	4	-1	67	68	7	4	-4	57	57	0	5	17	18	-12	3	5	-13	151	-150
1	4	-16	43	-41	4	4	-2	75	-64	7	4	-5	123	-114	0	5	18	56	49	3	5	-14	-19	7
1	4	-17	-23	-2	4	4	-3	64	61	7	4	-6	51	37	0	5	19	82	84	3	5	-15	80	-69
1	4	-18	50	-52	4	4	-4	147	149	7	4	-7	-26	-5	1	5	1	64	-67	3	5	-16	86	-76
1	4	-19	66	58	4	4	-5	-24	-12	7	4	-8	-26	10	1	5	2	-15	8	3	5	-17	202	172
1	4	-20	-16	9	4	4	-6	118	112	7	4	-9	-26	1	1	5	3	142	-144	3	5	-18	66	62
1	4	-21	47	-54	4	4	-7	234	-231	7	4	-10	-25	6	1	5	4	93	92	4	5	1	62	59
2	4	1	34	-23	4	4	-8	313	-347	7	4	-11	-25	22	1	5	5	-18	-2	4	5	2	186	-178
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2	4	3	30	-20	4	4	-10	138	137	7	4	-14	82	-76	1	5	7	97	79	4	5	4	83	72
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4	4	5	170	-170	7	4	3	30	-30	0	5	2	58	-42	3	5	14	44	36	6	5	-6	58	-50
4	4	6	52	-41	7	4	4	-26	3	0	5	3	148	155	3	5	15	131	109	6	5	-7	92	86
4	4	7	88	-64	7	4	5	30	-16	0	5	4	65	-69	3	5	16	55	-37	6	5	-8	-20	16
4	4	8	93	89	7	4	6	33	-23	0	5	5	142	148	3	5	17	136	-134	6	5	-9	-20	8
4	4	9	149	146	7	4	7	80	72	0	5	6	97	-91	3	5	-1	146	153	6	5	-10	-20	-17
4	4	10	58	-58	7	4	8	112	103	0	5	7	162	164	3	5	-2	141	-146	6	5	-11	163	-161
4	4	11	41	32	7	4	9	-24	3	0	5	8	84	-84	3	5	-3	52	-44	6	5	-12	68	61
4	4	12	138	-127	7	4	10	32	23	0	5	9	41	37	3	5	-4	31	-25	6	5	-13	29	234

Table 8. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
6	5-14		78	-70	9	5 -4		-14	-3	1	6-13		256	-219	3	6 -9		99	71	5	6-11		269	-290
6	5-15		134	-129	9	5 -5		40	-41	1	6-14		-30	-36	3	6-10		63	-51	5	6-12		-29	-8
6	5-16		23	21	9	5 -6		-13	1	1	6-15		229	213	3	6-11		50	-16	5	6-13		176	189
7	5 1		50	-45	9	5 -7		52	53	1	6-16		-23	1	3	6-12		-34	-13	5	6-14		37	-43
7	5 2		80	70	9	5 -8		81	85	1	6-17		-17	20	3	6-13		-31	5	5	6-15		33	-45
7	5 3		32	25	9	5 -9		-10	-14	2	6 1		94	94	3	6-14		-29	9	6	6 1		111	93
7	5 4		-19	15	1	6 0		33	-9	2	6 2		47	32	3	6-15		97	-76	6	6 2		-35	32
7	5 5		117	55	2	6 0		93	99	2	6 3		56	61	3	6-16		31	37	6	6 3		52	44
7	5 6		-18	-10	3	6 0		-35	5	2	6 4		-35	-5	4	6 1		137	123	6	6 4		-34	-28
7	5 7		244	-236	4	6 0		-37	-8	2	6 5		150	-172	4	6 2		-37	-30	6	6 5		57	49
7	5 8		-17	21	5	6 0		77	61	2	6 6		48	26	4	6 3		392	-448	6	6 6		-32	27
7	5 9		202	153	6	6 0		54	-32	2	6 7		201	222	4	6 4		72	-60	6	6 7		56	-61
7	5 10		-14	-2	7	6 0		36	32	2	6 8		-38	-18	4	6 5		151	145	6	6 8		-29	24
7	5 11		-13	-7	8	6 0		-25	26	2	6 9		111	-101	4	6 6		58	58	6	6 9		115	111
7	5 -1		75	-56	0	6 1		279	-347	2	6 10		-36	-30	4	6 7		78	66	6	6 10		-23	-6
7	5 -2		-20	6	0	6 2		70	-73	2	6 11		61	55	4	6 8		56	-46	6	6 11		87	-113
7	5 -3		246	255	0	6 3		161	188	2	6 12		47	39	4	6 9		73	-64	6	6 -1		164	-148
7	5 -4		-20	-13	0	6 4		50	52	2	6 13		53	-33	4	6 10		-33	-1	6	6 -2		-35	-40
7	5 -5		294	-265	0	6 6		88	103	2	6 14		-28	-8	4	6 11		62	-56	6	6 -3		236	199
7	5 -6		-15	-16	0	6 6		-35	-26	2	6 15		-24	41	4	6 12		-28	-15	6	6 -4		-35	19
7	5 -7		117	54	0	6 7		104	-106	2	6 16		-18	21	4	6 13		124	127	6	6 -5		109	-86
7	5 -8		-55	-45	0	6 8		42	46	2	6 -1		157	171	4	6 14		-19	-22	6	6 -6		59	54
7	5 -9		-18	13	0	6 9		141	-121	2	6 -2		-32	-17	4	6 -1		67	-62	6	6 -7		-33	-14
7	5-10		-17	21	0	6 10		-37	-25	2	6 -3		-33	16	4	6 -2		-37	14	6	6 -8		-32	-24
7	5-11		26	-29	0	6 11		242	204	2	6 -4		-34	7	4	6 -3		98	-84	6	6 -9		-31	-18
7	5-12		72	-70	0	6 12		85	74	2	6 -5		-35	-5	4	6 -4		-38	-31	6	6-10		41	34
7	5-13		76	-82	0	6 13		215	-178	2	6 -6		-36	31	4	6 -5		-38	12	6	6-11		109	109
7	5-14		21	-25	0	6 15		63	-57	2	6 -7		-37	-28	4	6 -6		58	47	6	6-12		27	29
7	5-15		111	149	0	6 15		109	96	2	6 -8		-38	-26	4	6 -7		115	83	6	6-13		116	-139
8	5 1		-18	-7	0	6 16		46	57	2	6 -9		-37	-17	4	6 -8		119	-90	7	6 1		65	-54
8	5 2		20	25	0	6 17		44	62	2	6-10		-37	-27	4	6 -9		250	-186	7	6 2		-31	-33
8	5 3		65	65	1	6 1		57	67	2	6-11		80	63	4	6-10		71	48	7	6 3		-30	30
8	5 4		62	-54	1	6 2		38	42	2	6-12		-34	0	4	6-11		143	105	7	6 4		-29	-13
8	5 5		132	-117	1	6 3		52	63	2	6-13		65	52	4	6-12		37	-42	7	6 5		-28	13
8	5 6		31	37	1	6 4		88	-115	2	6-14		46	27	4	6-13		51	-48	7	6 6		-26	-9
8	5 7		69	79	1	6 5		58	63	2	6-15		-27	12	4	6-14		-26	37	7	6 7		-24	34
8	5 8		60	64	1	6 6		36	-5	2	6-16		90	-77	4	6-15		-22	-30	7	6 -1		66	73
8	5 9		31	-34	1	6 7		113	-120	3	6 1		46	-39	5	6 1		155	-156	7	6 -2		58	60
8	5 10		-9	-3	1	6 8		37	-35	3	6 2		-36	-29	5	6 2		56	-43	7	6 -3		70	-70
8	5 -1		-18	-8	1	6 9		220	230	3	6 3		268	261	5	6 3		109	81	7	6 -4		36	-23
8	5 -2		90	-86	1	6 10		-37	38	3	6 4		-37	3	5	6 4		82	86	7	6 -5		-30	24
8	5 -3		95	-90	1	6 11		119	-102	3	6 5		121	-112	5	6 5		-36	-22	7	6 -6		98	101
8	5 -4		32	-25	1	6 12		68	-56	3	6 6		44	38	5	6 6		62	-44	7	6 -7		-29	22
8	5 -5		210	166	1	6 13		-32	21	3	6 7		-38	27	5	6 7		131	-121	7	6 -8		-27	0
8	5 -6		57	52	1	6 14		-30	5	3	6 8		-38	-25	5	6 8		-34	-4	7	6 -9		-25	-8
8	5 -7		222	-153	1	6 15		-26	26	3	6 9		56	43	5	6 9		109	-89	7	6-10		-22	-20
8	5 -9		85	80	1	6 16		-22	-10	3	6 10		-35	-14	5	6 10		-29	40	8	6 1		-25	7
8	5-10		-14	17	1	6 -1		252	-288	3	6 11		82	-63	5	6-11		178	179	8	6 2		-24	23
8	5-11		-13	12	1	6 -2		78	72	3	6 12		-31	-4	5	6 12		-23	26	8	6 3		56	63
8	5-12		46	45	1	6 -3		317	405	3	6 13		33	48	5	6 -1		205	182	8	6 4		-21	20
9	5 1		38	40	1	6 -4		46	31	3	6 14		46	19	5	6 -2		67	-43	8	6 -1		91	-117
9	5 2		66	-89	1	6 -5		-34	-15	3	6 -1		143	-149	5	6 -3		-37	-37	8	6 -1		57	-55
9	5 3		-13	-17	1	6 -6		80	85	3	6 -2		74	-71	5	6 -4		-37	13	8	6 -2		-25	15
9	5 4		42	47	1	6 -7		-37	17	3	6 -3		114	-110	5	6 -5		74	-49	8	6 -3		-25	3
9	5 5		50	53	1	6 -8		-37	-6	3	6 -4		-36	4	5	6 -6		74	-57	8	6 -4		-25	22
9	5 6		14	-17	1	6 -9		68	45	3	6 -5		120	93	5	6 -7		7	7	8	6 -5		72	78
9	5 -1		-15	-14	1	6-10		-37	22	3	6 -6		93	-85	5	6 -8		-36	3	8	6 -6		61	-66
9	5 -2		22	23	1	6-11		117	94	3	6 -7		132	-125	5	6 -9		165	150	8	6 -7		92	-104
9	5 -3		-14	13	1	6-12		60	57	3	6 -8		87	64	5	6-10		-34	20	8	6 -8		-17	11

An analysis of the thermal parameters of the S and C atoms, assuming the whole molecule a rigid body, was carried out according to the method of Schomaker and Trueblood.[5] The rigid-body tensors arrived at are given in Table 6. The translational tensor **T** and the screw tensor **S** are in Table 6 given relative to the unique origin which symmetrizes **S**. This origin lies about 0.40 Å from the center of gravity of the molecule, displaced along the three crystal axes by 0.16, 0.33, and 0.17 Å, respectively.

The r.m.s. difference between observed and calculated U_{ij}'s is 0.0044 Å.² The maximum and minimum translation amplitudes are 0.202 and 0.173 Å, respectively, and the translational motion is thus not markedly anisotropic. The maximum and minimum libration amplitudes are 3.9 and 1.5°, respectively, and this motion is thus somewhat more anisotropic. However, corrections in bond lengths for rigid-body libration of this order of magnitude are not great, as seen from the bond length values in the second column of Table 1.

Separate rigid-body analysis for certain parts of the 2-methyl-4-phenyl-thiothiophthene molecule have also been carried out. The parts of the molecule treated in this way are, the thiothiophthene system plus C(6) and C(7), and ring *C* plus C(4). The librational tensors from these calculations are listed in Table 7.

The rigid-body analysis of the mentioned parts of the molecule gave better fit between observed and calculated U_{ij}'s than did the rigid-body analysis of the entire molecule. Thus from the analysis of the thiothiophthene system plus C(6) and C(7), the r.m.s. difference of U_{ij}'s is 0.0035 Å², and similarly for ring *C* plus C(4), the r.m.s. difference is 0.0032 Å².

Bond lengths which have been corrected according to the libration tensors $\mathbf{L}_{(A+B)}$ and $\mathbf{L}_C$, respectively, are listed in the first column of Table 1.

The final list of structure factors is given in Table 8.

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