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The Crystal and Molecular Structure of 2,5-Diphenyl-thiothiophthene

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An X-ray structure study of crystals of 2,5-diphenyl-thiothiophthene has been carried out. The crystals belong to the orthorhombic space group $P2_12_12_1$, with unit cell dimensions $a=11.955$, $b=15.170$, and $c=7.915$ Å. 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 1667 $hk0-hk7$ and $0kl$ reflections.

Unequal S–S distances occur in the linear three sulphur sequence of the molecule, *i.e.* S(1)–S(2) = 2.362 ± 0.003 Å, S(2)–S(3) = 2.304 ± 0.003 Å, with the angle S(1)–S(2)–S(3) = 176.6 ± 0.1°. The other bond lengths in the thiothiophthene system are S(1)–C(1) = 1.712 ± 0.006 Å, S(2)–C(3) = 1.753 ± 0.006 Å, S(3)–C(5) = 1.703 ± 0.006 Å, C(1)–C(2) = 1.374 ± 0.009 Å, C(2)–C(3) = 1.413 ± 0.009 Å, C(3)–C(4) = 1.391 ± 0.009 Å, and C(4)–C(5) = 1.393 ± 0.008 Å.

The C–C bonds connecting the phenyl groups to the thiothiophthene system are C(1)–C(12) = 1.483 + 0.009 Å, and C(5)–C(6) = 1.486 ± 0.008 Å.

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

The thiothiophthene system is nearly planar, and the phenyl group bonded to C(5) is almost co-planar with the thiothiophthene system; the twist angle of this phenyl group about the connection bond C(5)–C(6) is 3.3°. The other phenyl group is not co-planar with the thiothiophthene system. It is twisted 45.1° about the connection bond C(1)–C(12).

In crystals of 2,5-diphenyl-thiothiophthene, S(3) approaches the plane of the thiothiophthene system in a symmetry-related molecule at a distance of 3.25 Å, with the bond S(3)–C(5) forming an angle of 77° with this plane.

There are unequal sulphur-sulphur distances in both of the unsymmetric thiothiophthene derivatives I and II.[1–3] Two sets of S–S bond lengths occur in II, corresponding to the two crystallographically independent mole-

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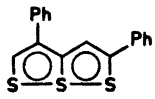
cules in the crystal structure. The sulphur – sulphur distances in the symmetric derivative III are found to be equal.[4–6]

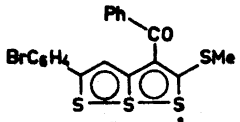
It has been pointed out by different authors [2,7] that the results from III could be ambiguous since they may represent the average of two-fold disorder of molecules with a "short" and a "long" S – S distance. The molecules lie in special positions, with crystallographic mirror plane passing through the central sulphur and carbon atoms, and the central sulphur atom shows a pronounced anisotropy which may indicate such disorder.

It has been suggested,[2] therefore, that the "short" S – S distance in the 2.12 – 2.22 Å range, and the "long" S – S distance in the range 2.47 – 2.57 Å are typical for the thiothiophthene system, irrespective of the substituents. The present structure study of the symmetric thiothiophthene derivative IV, for which both S – S distances could be independently determined, has been carried out in order to test this hypothesis.



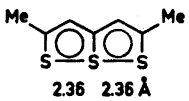
2.22 2.50 Å

(I)



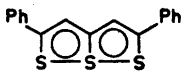
2.17 2.45 Å
2.16 2.56 "

(II)



2.36 2.36 Å

(III)



(IV)

STRUCTURE DETERMINATION

A brief account of the structure determination has been reported earlier,[8] and a more detailed description is given here.

Crystals of 2,5-diphenyl-thiothiophthene (IV) were generously supplied by Klingsberg.[9] The crystals are deep purple and belong to the orthorhombic space group $P2_12_12_1$.

Structure analysis is based on photographic data, taken with Weissenberg camera and Cu$K\alpha$ radiation. The data comprise 1667 $hk0 - hk7$ and $0kl$ reflections, including 182 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 atoms of the phenyl groups revealed themselves during a subsequent Fourier synthesis.

The structure refinement was carried out by Shino's version of the Busing, Martin and Levy full-matrix least-squares IBM 7090 program.[10,11] Anisotropic

temperature factors were applied to sulphur and carbon, and isotropic to hydrogen. The final R factor is 7.9 % when unobserved reflections are included, and 7.1 % when they are omitted.

A rigid-body analysis of the 2,5-diphenyl-thiothiophthene molecule has been carried out according to the method of Schomaker and Trueblood,[12] and the S–S, S–C, and C–C bond lengths have been corrected for rigid-body libration according to Cruickshank's formula.[13] For further details with respect to the structure determination, see Experimental.

Table 1. Bond lengths (l) and standard deviation in bond lengths $\sigma(l)$ in 2,5-diphenyl-thiothiophthene. Bond lengths (l') and (l'') with correction for rigid-body libration are given for the S–S, S–C and C–C bonds. 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 libration tensors one gets when the phenyl groups and the thiothiophthene system are treated separately. For further explanation, see the text.

Bond	l'' (Å)	l' (Å)	l (Å)	$\sigma(l)$ (Å)
S(1)–S(2)	2.362	2.363	2.360	0.003
S(1)–C(1)	1.712	1.710	1.702	0.006
S(2)–S(3)	2.304	2.305	2.302	0.003
S(2)–C(3)	1.753	1.750	1.743	0.006
S(3)–C(5)	1.703	1.701	1.694	0.006
C(1)–C(2)	1.374	1.374	1.371	0.009
C(1)–C(12)	1.483	1.482	1.479	0.009
C(2)–C(3)	1.413	1.413	1.410	0.009
C(3)–C(4)	1.391	1.391	1.388	0.009
C(4)–C(5)	1.393	1.393	1.391	0.008
C(5)–C(6)	1.486	1.485	1.482	0.008
C(6)–C(7)	1.420	1.407	1.404	0.009
C(6)–C(11)	1.380	1.371	1.364	0.010
C(7)–C(8)	1.395	1.394	1.391	0.011
C(8)–C(9)	1.367	1.358	1.351	0.011
C(9)–C(10)	1.431	1.418	1.415	0.012
C(10)–C(11)	1.380	1.378	1.376	0.011
C(12)–C(13)	1.408	1.404	1.400	0.010
C(13)–C(14)	1.404	1.402	1.399	0.012
C(14)–C(15)	1.360	1.355	1.349	0.012
C(15)–C(16)	1.416	1.412	1.407	0.012
C(16)–C(17)	1.403	1.401	1.398	0.011
C(17)–C(12)	1.399	1.394	1.387	0.009

Bond	l (Å)	Bond	l (Å)
C(2)–H(2)	0.95	C(11)–H(11)	1.08
C(4)–H(4)	0.85	C(13)–H(13)	0.91
C(7)–H(7)	0.99	C(14)–H(14)	1.04
C(8)–H(8)	0.84	C(15)–H(15)	0.98
C(9)–H(9)	0.94	C(16)–H(16)	0.79
C(10)–H(10)	1.08	C(17)–H(17)	1.20

The standard deviation in C–H bond lengths is estimated to be 0.08 Å.

Table 2. Bond angles ∠(ijk) in 2,5-diphenyl-thiothiophthene. The standard deviations given in parentheses refer to the last digits of respective values.

i	j	k	∠(ijk)°	i	j	k	∠(ijk)°
C(1)	S(1)	S (2)	93.2 (2)	C(5)	C(6)	C(7)	120.1 (5)
S(1)	C(2)	S (3)	176.6 (1)	C(5)	C(6)	C(11)	121.8 (6)
S(1)	S(2)	C (3)	89.2 (2)	C(7)	C(6)	C(11)	118.0 (6)
C(3)	S(2)	S (3)	89.0 (2)	C(6)	C(7)	C(8)	120.3 (6)
S(2)	S(3)	C (5)	94.8 (2)	C(7)	C(8)	C(9)	121.2 (7)
S(1)	C(1)	C (2)	117.3 (5)	C(8)	C(9)	C(10)	118.7 (8)
S(1)	C(1)	C(12)	118.9 (5)	C(9)	C(10)	C(11)	119.7 (8)
C(2)	C(1)	C(12)	123.8 (6)	C(10)	C(11)	C(6)	122.0 (7)
C(1)	C(2)	C (3)	121.9 (6)	C(1)	C(12)	C(13)	120.0 (6)
C(2)	C(3)	S (2)	118.3 (5)	C(1)	C(12)	C(17)	119.8 (6)
C(2)	C(3)	C (4)	122.3 (6)	C(13)	C(12)	C(17)	120.2 (6)
S(2)	C(3)	C (4)	119.4 (5)	C(12)	C(13)	C(14)	118.3 (7)
C(3)	C(4)	C (5)	120.7 (6)	C(13)	C(14)	C(15)	121.4 (8)
C(4)	C(5)	S (3)	116.0 (5)	C(14)	C(15)	C(16)	121.4 (8)
C(4)	C(5)	C (6)	124.5 (5)	C(15)	C(16)	C(17)	117.6 (7)
S(3)	C(5)	C (6)	119.5 (4)	C(16)	C(17)	C(12)	121.0 (6)

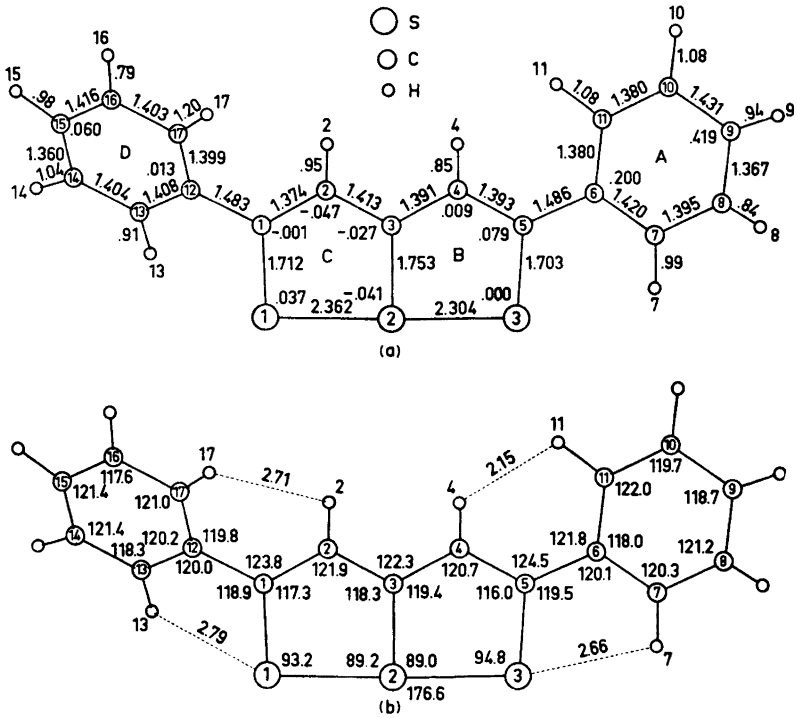


Fig. 1. (a) Bond lengths (Å) in the 2,5-diphenyl-thiothiophthene molecule, and atomic distances (Å) from the least squares plane of the thiothiophthene system. (b) Bond angles (°) and intramolecular non-bonding distances (Å).

DISCUSSION

Molecular shape and dimensions. Bond lengths and angles in the 2,5-diphenyl-thiothiophthene molecule, together with their standard deviations, are listed in Tables 1 and 2, and shown in Figs. 1a and 1b, respectively.

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, with triple weight on sulphur, is

$$0.53177\,X - 0.20521\,Y + 0.82165\,Z = 2.48163$$

with X, Y, and Z in Å units. Deviations from the plane for the atoms of the thiothiophthene system the atoms C(6) and C(9) of phenyl group A, and the atoms C(12) and C(15) of phenyl group D, are given in Fig. 1a. It is seen that the thiothiophthene system is almost planar. The linear sequence C(5) – C(6) – C(9) points slightly out of the plane of the thiothiophthene system and the sequence C(1) – C(12) – C(15) lies almost in the plane.

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

$$0.53686\,X - 0.11466\,Y + 0.83585\,Z = 2.90363$$

and the deviations in Å units from this plane are C(6) – 0.015, C(7) 0.012, C(8) 0.001, C(9) – 0.010, C(10) 0.006, and C(11) 0.006.

Similarly the equation for the plane of phenyl group D is

$$-0.24564\,X - 0.38732\,Y + 0.88862\,Z = -2.99196$$

with deviations C(12) – 0.006, C(13) 0.000, C(14) 0.000, C(15) 0.006, C(16) – 0.012, and C(17) 0.012 Å.

The twist angle about C(5) – C(6) of phenyl group A is 3.3°, and A is thus almost co-planar with the thiothiophthene system. The twist angle was taken as the angle between the normal to the plane through S(3), C(4), C(5), and C(6), and the normal to the plane through C(5), C(6), C(7), and C(11).

Similarly, the twist angle of phenyl group D, about C(1) – C(12), was found to be 45.1°.

Comparison with the structure of 2,5-dimethyl-thiothiophthene. The molecular structure of 2,5-dimethyl-thiothiophthene has recently been reinvestigated by Leung and Nyburg.[14] The structure study was based on diffractometer data (Cu$K\alpha$ radiation) which were corrected for absorption, and the refinement was carried out by means of a full matrix least squares procedure. Furthermore, the structure was refined in both space group *Pnma* and space group $Pn2_1a$. Leung and Nyburg conclude from the results of the refinement in space group *Pnma* that "there is no *prima facie* evidence for statistical disordering in this structure or, if there is disordering, the differences in the two molecular geometries is too small to be detected by X-ray structure analysis." Bond lengths in 2,5-dimethyl-thiothiophthene from the refinement in space group *Pnma* are given in Fig. 2, and corresponding bonds in 2,5-dimethyl- and 2,5-diphenyl-thiothiophthene may now be compared.

The sulphur-sulphur bond lengths in 2,5-diphenyl-thiothiophthene (*cf.* Fig. 1a) are S(1) – S(2) = 2.362 ± 0.003 Å, and S(2) – S(3) = 2.304 ± 0.003 Å,

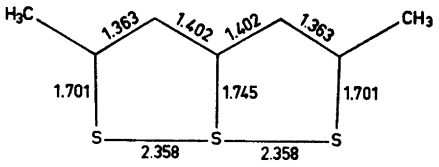


Fig. 2. Bond lengths (Å) in 2,5-dimethyl-thiothiophthene.

respectively. The difference in S – S bond length, 0.058 Å, corresponds to 14 standard deviations, and is therefore significant. In 2,5-dimethyl-thiothiophthene, both S – S bonds are 2.358 ± 0.001 Å (*cf.* Fig. 2).

The lengths of the carbon-sulphur bonds in the two compounds agree closely. They are 1.712, 1.753, and 1.703 ± 0.006 Å in the diphenyl derivative, and 1.701, 1.745, and 1.701 ± 0.004 Å in the dimethyl derivative, reckoned in the same order. The latter values have not been corrected for libration. In the present study, the uncorrected C – S bond lengths are 1.702, 1.743, and 1.694 ± 0.006 Å, respectively (*cf.* Table 1).

The sum of the S – S bond lengths in 2,5-dimethyl-thiothiophthene, 4.716 Å, is 0.050 Å greater than the sum of the S – S bond lengths in 2,5-diphenyl-thiothiophthene, 4.666 Å. The difference of 0.050 Å represents 16.7σ, if one takes σ equal to 0.003 Å, as obtained for the S – S bonds in the present investigation.

Structural analogy between thiothiophthene and naphthalene. Thiothiophthene and naphthalene are analogous compounds as far as their π-bonding systems are concerned; there is a 10 π-electron system in both.

The molecular structure of naphthalene has been studied by Cruickshank,[15] and the C – C bond lengths of interest for the present discussion are given in Fig. 3. It is seen there that the two central C – C bond lengths are longer

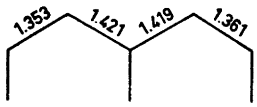


Fig. 3. Bond lengths (Å) in naphthalene.

than the adjacent terminal ones; the central bonds are 1.421 and 1.419 ± 0.005 Å, and the terminal bonds are 1.353 and 1.361 ± 0.005 Å, respectively. Such a difference between central and terminal C – C bonds occur also in the thiothiophthene system of the thiothiophthene derivatives which so far have been studied.[1–6,16–20] In 2,5-dimethyl-thiothiophthene for example (*cf.* Fig. 2), the central and terminal C – C bonds are 1.402 and 1.363 ± 0.004 Å, respectively. In the present structure, the average central and terminal C – C bonds are 1.402 and 1.384 ± 0.009 Å, respectively.

The crystal structure. The arrangement of 2,5-diphenyl-thiothiophthene molecules in the unit cell, as seen along the *a*-axis and along the *c*-axis, is shown in Figs. 4a and 4b, respectively. One should note the way in which the molecule in position II is arranged relative to the reference molecule I. Molecule II lies *c*/2 above I, and the plane of the thiothiophthene system in II, and that of the thiothiophthene system in I are nearly perpendicular to each

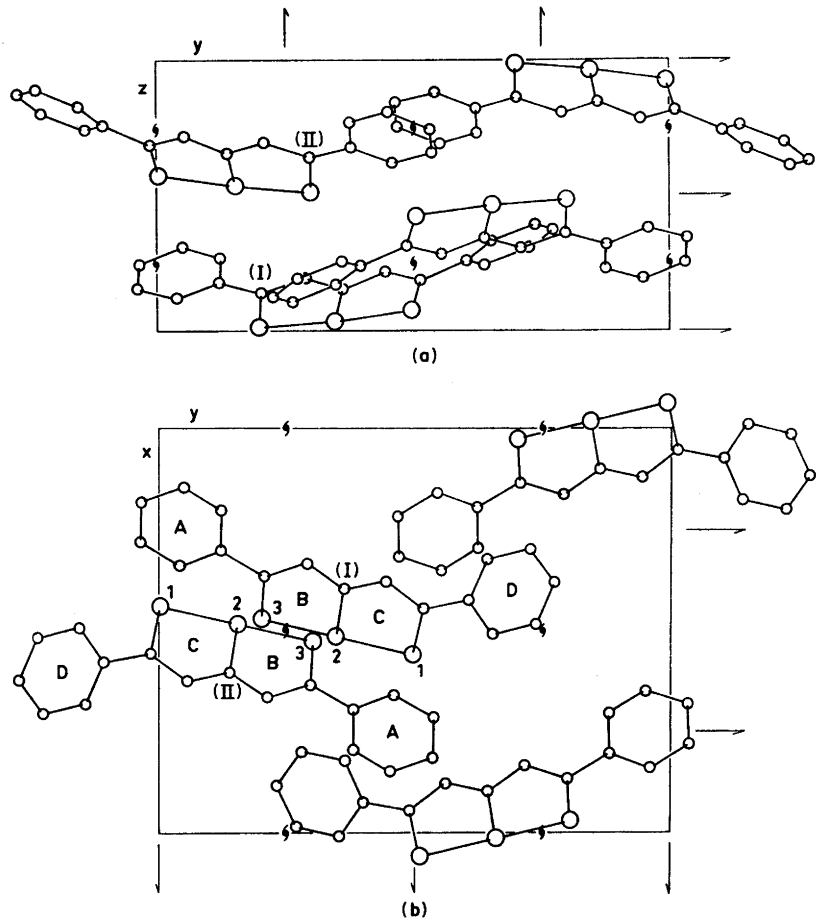


Fig. 4. The arrangement of 2,5-diphenyl-thiothiophthene molecules as seen along the *a*-axis (a), and along the *c*-axis (b).

other. There is a contact of 3.25 Å between S(3) in II and the plane of ring *B* in the reference molecule. This contact is 0.30 Å shorter than the sum of the van der Waals radius for sulphur, 1.85 Å, and the half-thickness of an aromatic molecule, 1.70 Å.[21] The C(5)–S(3) bond in II forms an angle of 77° with the plane of ring *B* in I.

The mentioned close contact in 2,5-diphenyl-thiothiophthene is comparable with a corresponding close contact present in crystals of the benzene-chlorine (1:1) charge-transfer complex.[22] There, the chlorine molecules are arranged perpendicular to the planes of the benzene molecules, and the distance from a chlorine atom to the nearest benzene plane is 3.28 Å, as compared with the corresponding van der Waals distance of 3.50 Å.

S(1) and S(2) do not form close contacts with neighbouring molecules.

Conclusion. It has been shown that in the crystal structure of 2,5-diphenylthiothiophthene, the two sulphur – sulphur bonds are of different lengths, although the molecule is symmetric with respect to substituents. The difference in S – S bond length, 0.058 Å, may be explained if one takes into account that the twist of the phenyl substituents about the respective connection bonds are different, and that S(3) forms close contact with the plane of the thiothiophthene system of a symmetry-related molecule.

From the spatial orientation of phenyl groups *A* and *D*, the conjugation across C(5) – C(6) must be more pronounced than the conjugation across C(1) – C(12). The π-bonding in the thiothiophthene system, therefore, is unsymmetrically perturbed, and this may affect the bonding in the three-sulphur sequence. Furthermore, if the close contact in which S(3) is involved is established through a transfer of negative charge towards S(3), the atom might become less electronegative than S(1). One should then, by reference to

Table 3. Atomic coordinates in fractions of corresponding cell edges. The standard deviations given in parentheses for sulphur and carbon refer to the last digits of respective values.

Atom	*x*	*y*	*z*
S(1)	0.56153 (16)	0.49581 (10)	0.07487 (27)
S(2)	0.51774 (14)	0.34598 (10)	0.03393 (24)
S(3)	0.47521 (15)	0.19880 (10)	0.01122 (25)
C(1)	0.44496 (54)	0.51474 (37)	0.19235 (88)
C(2)	0.37505 (51)	0.44487 (36)	0.22033 (89)
C(3)	0.39930 (48)	0.35991 (36)	0.15893 (85)
C(4)	0.33252 (50)	0.28771 (37)	0.19511 (88)
C(5)	0.36137 (48)	0.20432 (34)	0.13765 (82)
C(6)	0.29902 (48)	0.12279 (33)	0.17817 (82)
C(7)	0.33868 (60)	0.04096 (37)	0.12202 (104)
C(8)	0.27959 (74)	−0.03555 (39)	0.15772 (117)
C(9)	0.18439 (73)	−0.03342 (47)	0.24926 (108)
C(10)	0.14588 (70)	0.04853 (45)	0.31076 (128)
C(11)	0.20428 (67)	0.12404 (45)	0.27383 (106)
C(12)	0.42447 (55)	0.60442 (38)	0.25768 (83)
C(13)	0.51120 (63)	0.65147 (43)	0.33427 (116)
C(14)	0.48847 (84)	0.73595 (52)	0.39548 (109)
C(15)	0.38566 (81)	0.77150 (42)	0.38317 (110)
C(16)	0.29728 (73)	0.72594 (43)	0.30535 (120)
C(17)	0.31858 (56)	0.64086 (40)	0.24650 (94)
H(2)	0.3102	0.4460	0.2895
H(4)	0.2843	0.2924	0.2734
H(7)	0.3975	0.0356	0.0346
H(8)	0.2956	−0.0845	0.1136
H(9)	0.1572	−0.0899	0.2747
H(10)	0.0676	0.0487	0.3772
H(11)	0.1720	0.1851	0.3245
H(13)	0.5793	0.6261	0.3219
H(14)	0.5588	0.7652	0.4880
H(15)	0.3654	0.8290	0.4470
H(16)	0.2182	0.7427	0.3130
H(17)	0.2650	0.6151	0.2160

the bonding in the linear trihalide ions,[24-27] expect S(1) – S(2) to be longer than S(2) – S(3), in agreement with the experimental results. It might be mentioned in this connection that the bond C(5) – S(3) of molecule II points towards that part of the thiothiophthene system in molecule I, where its π-electron density from MO calculation, is greatest (*cf.* Fig. 4, and Refs. 1 and 23).

The potential energy of the three-center bond in thiothiophthene as a function of the displacement of the central sulphur atom from the symmetrical location toward the terminal sulphur atoms has been calculated by Gleiter and Hoffmann.[28] The energy curve for three-center bonds formed by combination of sulphur 3*p*-orbitals as well as sulphur 3*d*-orbitals has a flat and broad (about 0.3 Å) minimum about the symmetrical structure. The results from the present investigation supports this description of the three-center bond in thiothiophthene.

EXPERIMENTAL

The unit cell dimensions for crystals of 2,5-diphenyl-thiothiophthene were determined from high order reflections on *hk*0 and 0*kl* Weissenberg photographs. The cell dimensions found in this way, $a = 11.955$, $b = 15.170$, and $c = 7.915$ Å, are believed to be within ± 0.2 % of the correct values. Four molecules per unit cell give a calculated density of 1.446 g/cm^3 as compared with the density 1.44 g/cm^3 found by flotation.

The intensities of the *hk*0 – *hk*7 and 0*kl* reflections were estimated visually. Small crystals were used in order to minimize absorption effects, and no absorption correction was applied. The intensities were correlated and reduced to the structure amplitudes by means of an IBM 7090 program,[29] which uses the procedure by Hamilton *et al.*[30]

Table 4. Temperature parameters $\beta_{ij} \times 10^4$ for sulphur and carbon. The expression used is $\exp -(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})$. The standard deviations in parentheses refer to the last digits of respective values.

	$\beta_{11} \times 10^4$	$\beta_{22} \times 10^4$	$\beta_{33} \times 10^4$	$\beta_{12} \times 10^4$	$\beta_{13} \times 10^4$	$\beta_{23} \times 10^4$
S(1)	86 (1)	38 (1)	200 (4)	−5 (1)	37 (2)	22 (1)
S(2)	74 (1)	37 (1)	132 (3)	5 (1)	32 (2)	14 (1)
S(3)	88 (1)	35 (1)	146 (3)	7 (1)	44 (2)	−1 (1)
C(1)	73 (5)	35 (2)	106 (12)	−10 (3)	−11 (6)	7 (4)
C(2)	63 (4)	32 (2)	134 (13)	5 (3)	−6 (6)	5 (4)
C(3)	58 (4)	34 (2)	90 (11)	2 (2)	−2 (5)	1 (4)
C(4)	63 (4)	35 (2)	101 (12)	3 (2)	1 (6)	3 (4)
C(5)	62 (4)	30 (2)	95 (11)	6 (2)	−15 (5)	1 (4)
C(6)	71 (4)	29 (2)	68 (10)	6 (2)	−15 (5)	−7 (4)
C(7)	95 (5)	29 (2)	170 (15)	10 (3)	10 (7)	−4 (5)
C(8)	134 (7)	26 (2)	168 (16)	0 (3)	−2 (9)	−2 (5)
C(9)	125 (7)	36 (3)	145 (15)	−16 (4)	10 (9)	−18 (5)
C(10)	104 (6)	43 (3)	213 (19)	−17 (4)	36 (9)	−20 (6)
C(11)	101 (6)	35 (3)	181 (17)	−12 (4)	42 (8)	−24 (5)
C(12)	82 (5)	33 (2)	90 (11)	−7 (3)	−1 (6)	18 (4)
C(13)	101 (6)	40 (3)	189 (15)	−22 (3)	−13 (8)	11 (6)
C(14)	134 (8)	49 (4)	126 (15)	−40 (5)	−13 (9)	−9 (6)
C(15)	149 (8)	33 (3)	149 (16)	−23 (4)	2 (9)	−16 (5)
C(16)	114 (7)	34 (3)	201 (17)	−6 (4)	15 (9)	−5 (6)
C(17)	77 (5)	28 (2)	154 (13)	−4 (3)	−12 (6)	−3 (4)

For the hydrogen atoms, a temperature factor $\exp[-3(\sin^2\theta/\lambda^2)]$ was used.

The scattering factors used for sulphur and carbon in the structure factor calculations were those given by Cromer and Waber.[31] For hydrogen, the scattering factor curve given by Stewart *et al.*[32] was used.

Hughes' weighting scheme, with $F_{min} = 3.0$, was used in the least squares refinement.[10] The hydrogen atoms were not included in the calculations until a refinement of the sulphur and carbon positions with isotropic temperature factors for both kinds of atoms had converged. All the hydrogen atoms in the molecule are bonded to sp^2-hybridized carbon, and their positions could therefore be estimated by assuming a C–H distance of 1.05 Å and C–C–H angles of 120°. Constant isotropic temperature factors $\exp-[3(\sin^2\theta/\lambda^2)]$ were applied to the hydrogen atoms. In the last refinement cycles, positional parameters for S, C, and H, and anisotropic temperature parameters for S and C were refined. The final atomic coordinates are listed in Table 3, and the temperature parameters are listed in Table 4. The final list of structure factors are given in Table 7.

Table 5. Results from the rigid-body analysis of the 2,5-diphenyl-thiothiophthene molecule.

	Eigenvalues	Eigenvectors (direction cosines × 10^4 relative to *a*, *b*, and *c*, respectively)		
Librational tensor, **L**	25.3 (°)²	−1547	−9854	−700
	4.6	−1069	−537	9928
	1.5	−9821	1611	−968
Translational tensor, **T**	0.0415 Å²	9789	819	−1871
	0.0371	−647	9932	960
	0.0279	1936	−818	9776

Symmetrized screw tensor **S**:

$$\begin{pmatrix} -361 & -131 & 46 \\ & 194 & 6 \\ & & 167 \end{pmatrix} \times 10^5 \text{ rad. Å}$$

Centre of gravity of the molecule is at $x = 0.39007$, $y = 0.35967$, $z = 0.19782$.
The origin which symmetrizes **S** is at $x = 0.35592$, $y = 0.35077$, $z = 0.19782$.

Table 6. Librational tensors from the rigid-body analysis of certain parts of the 2,5-diphenyl-thiothiophthene molecule. $\mathbf{L}_A$ refer to ring A plus C(5), $\mathbf{L}_{C+B}$ refer to the thiothiophthene system plus C(5) and C(12), and $\mathbf{L}_D$ refer to ring D plus C(12).

	Eigenvalues	Eigenvectors (direction cosines × 10^4 relative to *a*, *b*, and *c*, respectively)		
$\mathbf{L}_A$	83.0 (°)²	−4292	−8446	3200
	10.7	−572	3792	9235
	5.9	−9014	3782	−2108
$\mathbf{L}_{(C+B)}$	34.0	1648	9858	330
	3.0	1264	−543	9905
	−1.4	9782	−1590	−1333
$\mathbf{L}_D$	45.8	1500	9828	1081
	10.9	1613	−1322	9780
	2.6	9755	−1293	−1782

Table 7. Observed and calculated structure factors for 2,5-diphenyl-thiothiophthene. The values given are ten times the absolute values. The columns are: Index, $|F_{obs}|$, $|F_{cal}|$, A_{cal}, B_{cal}. Unobserved reflections are marked with asterisks.

L= 0 H= 2
909 916 916 0
L= 0 H= 4
0 390 384 384 0
L= 0 H= 6
0 566 546 546 0
L= 0 H= 8
0 124 103 103- 0
L= 0 H= 10
0 58 48 48 0
L= 0 H= 12
0 34* 23 23- 0
L= 0 H= 14
0 26 23 23 0
L= 0 H= 0
2 74 68 68- 0
4 563 503 503 0
6 844 788 788 0
8 396 332 332 0
10 30* 30 30- 0
12 248 262 262- 0
14 237 256 256 0
16 37 45 45- 0
18 25* 12 12 0
L= 2 H= 0
0 502 526 526- 0
L= 4 H= 0
0 337 366 366 0
L= 6 H= 0
0 159 159 159 0
L= 8 H= 0
0 54* 45 45 0
L= 0 H= 1
1 618 603 0 603-
2 601 589 589- 0
3 15* 16 0 16
4 215 206 206 0
5 427 415 0 415
6 368 317 317 0
7 724 673 0 673-
8 50 44 44 0
9 193 189 0 189
10 137 135 135- 0
11 109 107 0 107-
12 48 43 43- 0
13 195 165 0 165
14 81 75 75 0
15 101 100 0 100-
16 33* 31 31- 0
17 44 51 0 51-
18 35 43 43- 0
19 88 102 0 102
L= 1 H= 2
1 213 200 0 200
2 404 398 398- 0
3 128 106 0 106-
4 162 142 142 0
5 593 582 0 582-
6 766 745 745 0
7 110 105 0 105-
8 63 60 60 0
9 185 176 0 176-
10 210 192 192 0
11 244 233 0 233-
12 391 368 368 0
13 50 62 0 62-
14 224 235 235 0
15 64 63 0 63-
16 32* 21 21 0
17 29* 15 0 15-
18 24* 9 0 0
19 18* 27 0 27-
L= 0 H= 3
1 430 408 0 408-
2 80 76 76- 0
3 133 128 0 128
4 116 111 111- 0
5 649 567 0 567
6 501 476 476- 0
7 162 160 0 160-
8 175 144 144- 0
9 62 56 0 56
10 50 43 43 0
11 78 74 0 74
12 295 281 281- 0
13 56 49 0 49
14 43 57 57- 0
15 96 94 0 94-
16 71 84 84- 0
17 28* 18 0 18-
18 60 72 72 0
19 35 49 0 49
L= 0 H= 4
1 481 481 0 481-
2 516 486 486- 0
3 267 235 0 235
4 224 224 224- 0
5 728 646 0 646-
6 422 391 391 0
7 159 146 0 146-
8 99 89 89 0
9 177 160 0 160-
10 32* 4 4 0
11 48 39 0 39-
12 120 123 123 0
13 186 201 0 201-
14 35* 35 35 0
15 149 168 0 168-
16 50 58 58- 0
17 27* 4 0 4
18 41 51 51- 0
L= 0 H= 5
1 226 223 0 223-
2 350 316 316- 0
3 98 87 0 87
4 273 265 265 0
5 108 99 0 99
6 109 105 105- 0
7 150 143 0 143-
8 88 78 78 0
9 182 183 0 183
10 33* 31 31- 0
11 72 75 0 75-
12 95 93 93- 0
13 35* 30 0 30-
14 85 92 92- 0
15 32* 5 0 5-
16 76 84 84- 0
17 42 48 0 48
18 18* 32 32- 0
L= 0 H= 6
1 450 407 0 407-
2 564 531 531- 0
3 59 55 0 55
4 156 161 161- 0
5 180 160 0 160-
6 120 112 112 0
7 235 212 0 212-
8 282 296 296- 0
9 121 135 0 135
10 217 218 218- 0
11 88 87 0 87-
12 164 181 181- 0
13 35* 11 0 11-
14 84 54 54 0
15 129 144 0 144-
16 126 127 127- 0
17 22* 17 0 17
L= 0 H= 7
1 355 348 0 348-
2 557 476 476- 0
3 28* 23 0 23-
4 272 253 253 0
5 37 33 0 33
6 31 26 26- 0
7 119 111 0 111-
8 153 160 160- 0
9 77 74 0 74
10 56 66 66- 0
11 50 61 0 61-
12 60 77 77 0
13 44 53 0 53
14 27 34 34 0
15 34 33 0 33-
16 52 64 64- 0
17 34 50 0 50
L= 0 H= 8
1 185 165 0 165-
2 430 384 384- 0
3 421 410 0 410
4 202 179 179- 0
5 117 119 0 119-
6 101 94 94- 0
7 59 52 0 52-
8 319 314 314- 0
9 50 47 0 47
10 208 213 213- 0
11 35* 1 0 1
12 44 39 39- 0
13 31* 2 0 2
14 29* 2 2 0
15 63 70 0 70-
16 66 81 81- 0
L= 0 H= 9
1 46 44 0 44-
2 132 122 122- 0
3 116 108 0 108-
4 250 235 235 0
5 189 176 0 176
6 215 192 192- 0
7 35* 13 0 13-
8 59 56 56- 0
9 35* 19 0 19-
10 75 89 89 0
11 74 73 0 73
12 31* 4 4 0
13 28* 33 0 33
14 25* 30 30 0
15 20* 11 0 11-
L= 0 H= 10
1 90 89 0 89-
2 215 202 202- 0
3 426 396 0 396
4 272 263 263- 0
5 100 103 0 103-
6 43 46 46- 0
7 35* 35 0 35
8 49 49 49 0
9 34* 16 0 16
10 150 165 165- 0
11 48 58 0 58
12 37 43 43- 0
13 27 28 0 28
14 20* 5 5- 0
L= 0 H= 11
1 35* 17 0 17
2 137 116 116- 0
3 43 39 0 39-
4 253 248 248 0
5 35* 6 0 6-
6 34* 29 29 0
7 34* 32 0 32-
8 59 58 58 0
9 58 67 0 67-
10 25 22 22 0
11 26* 1 0 1-
12 23* 32 32 0
L= 0 H= 12
1 34* 8 0 8
2 34* 24 24- 0
3 174 173 0 173
4 33* 32 32- 0
5 33* 19 0 19
6 32* 21 21 0
7 43 46 0 46
8 29* 7 7 0
9 68 74 0 74
10 24* 31 31- 0
L= 0 H= 13
1 31* 19 0 19
2 31 43 43- 0
3 3C 42 0 42
4 47 54 54 0
5 29* 1 0 1
6 27* 7 7- 0
7 26* 4 0 4
8 39 47 47- 0
9 21* 10 0 10-
10 60 64 64 0
L= 0 H= 14
1 35 38 0 38-
2 47 53 53 0
3 52 68 0 68
4 30 32 32 0
5 23* 14 0 14-
6 21* 7 7- 0
L= 0 H= 15
1 31 44 0 44
2 41 66 66- 0
L= 1 H= 1
0 169 181 0 181
L= 1 H= 2
0 906 916 916 0
L= 1 H= 3
0 270 274 0 274-
L= 1 H= 4
0 287 287 287- 0
L= 1 H= 5
0 280 272 0 272-
L= 1 H= 6
0 99 102 102- 0
L= 1 H= 7
0 36 25 0 25-
L= 1 H= 8
0 93 95 95- 0
L= 1 H= 9
0 64 55 0 55
L= 1 H= 10
0 29* 4 4- 0
L= 1 H= 11
0 65 58 0 58
L= 1 H= 12
0 34 23 23 0
L= 1 H= 13
0 36 35 0 35
L= 1 H= 14
0 30 13 13- 0
L= 1 H= 15
0 15* 5 0 5-
L= 1 H= 0
1 272 263 0 263-
2 348 353 0 353-
3 428 419 0 419
4 228 208 0 208-
5 181 171 0 171-
6 580 548 0 548
7 355 346 0 346-
8 561 571 0 571-
9 230 198 0 198-
10 27* 11 0 11-
11 112 102 0 102-
12 297 289 0 289
13 352 390 0 398-
14 291 327 0 327-
15 97 94 0 94-
16 46 43 0 43
17 24* 15 0 15-
18 20* 16 0 16
19 81 87 0 87-
L= 1 H= 1
1 498 491 459 175-
2 142 143 141 2C
3 425 440 381 220-
4 171 161 64- 148-
5 168 160 36- 155
6 91 82 80- 21-
7 897 860 860 23-
8 220 186 68- 173-
9 141 130 5- 130
10 93 82 81 16-
11 60 63 52 37-
12 271 233 142 185-
13 529 489 453 185
14 88 74 48 57-
15 117 123 58- 109
16 27* 24 11 22-
17 63 79 75 24-
18 60 67 7- 67-
19 64 77 75 19-
L= 1 H= 2
1 1158 1167 580 1013-
2 558 574 475- 322-
3 281 289 185- 222-
4 90 83 67- 48-
5 202 193 192 17
6 609 584 187- 553
7 489 430 38 428-
8 493 462 13- 462-
9 134 115 108- 39-
10 40 29 27- 10
11 104 92 91 14
12 328 310 170- 259
13 146 150 143- 46
14 261 258 42 255-
15 80 82 77- 27
16 69 72 54- 48
17 23* 22 20- 10-
18 20* 14 4- 13
19 33 43 40- 14-
L= 1 H= 3
1 505 513 510 56-
2 474 490 83 483-
3 298 292 292 15-
4 248 243 37 240-
5 232 219 142- 166-
6 264 256 165 195-
7 594 586 528 255-
8 362 332 80- 322-
9 194 176 173- 33-
10 41 46 37- 27
11 131 123 57- 139
12 227 215 31- 212-
13 250 228 177 144
14 65 57 14- 55-
15 96 95 95- 7
16 26* 29 28- 8-
17 32 36 14 33
18 76 86 13 85-
L= 1 H= 4
1 58 53 39- 36
2 297 304 194 234-
3 222 215 197- 86
4 142 127 119- 59
5 258 245 66 236-
6 219 218 146- 162
7 77 68 34- 59
8 287 269 36- 266-
9 234 231 231- 6
10 33 30 14- 26-
11 44 40 34 22
12 226 220 20 219
13 127 120 37- 114-
14 267 281 163- 229-
15 109 118 103- 58
16 63 86 1- 86
17 37 40 36 17
18 45 51 25- 44
L= 1 H= 5
1 329 326 206- 253
2 351 374 203 314-
3 131 125 67- 106
4 115 108 40- 101-
5 370 388 255- 292
6 231 217 53 210-
7 262 266 211 162
8 289 294 96 278-
9 264 256 256- 11
10 124 115 93 67
11 57 66 1- 66
12 239 239 154- 183-
13 129 116 116 7-
14 101 103 11 102-
15 82 83 82- 11-
16 23* 1 0 1
17 54 47 33- 35-
18 77 81 30 75-
L= 1 H= 6
1 331 291 34- 289
2 78 68 6- 68-
3 332 327 191- 266
4 99 92 28 88
5 46 49 49 4
6 221 215 96- 193
7 107 103 73- 72
8 132 129 26 127-
9 254 249 239- 69
10 81 70 22 66
11 172 165 140 89
12 184 183 6 183
13 122 114 22- 111-
14 163 170 74- 153-
15 110 116 115- 19
16 65 73 20- 70
17 57 66 63 21
L= 1 H= 7
1 145 144 141- 28
2 189 195 63- 184-
3 259 260 243- 91
4 172 158 111- 113
5 282 291 289- 32-
6 127 124 8 124-
7 97 84 59 60
8 209 203 41 199-
9 224 224 203- 95
10 199 184 10- 184
11 145 142 117- 80-
12 162 167 21 166-
13 39 20 20 1
14 59 58 5- 57-
15 100 120 113- 38
16 40 56 43 36
17 27 34 24- 24
L= 1 H= 8
1 71 77 50 58
2 120 114 44- 105-
3 174 158 147- 60
4 124 117 117 1
5 300 293 235 176
6 152 156 10- 156
7 116 115 113 19-
8 191 172 54- 164-
9 267 267 205- 172
10 119 109 92 58
11 212 214 191 98
12 98 95 5- 95
13 68 62 23- 58
14 46 50 14 48-
15 87 85 75- 39
16 47 56 33 46
L= 1 H= 9
1 111 99 88- 46-
2 98 98 87- 46-
3 194 185 184- 23-
4 271 234 123- 199
5 225 209 152- 143-
6 29* 32 28 15-
7 101 87 17- 85-
8 164 164 111- 121-
9 186 193 190- 37
10 224 230 36- 227
11 90 94 90- 26-
12 88 89 9- 89-
13 33 28 24- 14
14 28 7 5 5
15 59 64 64- 4-
L= 1 H= 10
1 61 56 40 40
2 126 121 74 96-
3 170 148 120- 88
4 180 169 150 78
5 128 128 128 12
6 29* 8 0 8
7 54 53 9 52
8 57 67 32- 59-
9 156 165 138- 90
10 46 35 24 22
11 145 153 138 66
12 39 40 14 37
13 20* 23 11- 20-
14 16* 27 14- 23-
L= 1 H= 11
1 29* 13 13- 1
2 92 80 51 62
3 166 157 113- 109-
4 135 131 59 117
5 57 63 13- 62
6 40 33 1 33
7 58 49 27- 41
8 39 41 40 11-
9 71 65 62- 20-

Table 7. Continued.

10	144	168	0	168
11	37	42	21-	36-
12	43	45	23-	39-
13	20	29	29-	4-
	L= 1 H= 12			
1	28*	19	8	17-
2	48	56	6	55-
3	100	110	57-	94
4	82	77	10	77
5	84	90	86	28
6	26*	16	7	14-
7	25*	17	6-	16-
8	52	46	46	5
9	69	73	45-	58-
10	27	6	6-	0
11	91	96	95	13
	L= 1 H= 13			
1	25*	12	9	8
2	36	43	22	36
3	25*	40	25-	31
4	83	94	4	94
5	33	30	28	13-
6	22*	12	4-	12
7	21*	15	8	13-
8	19*	10	10-	3
9	16*	9	9	1-
10	83	97	18-	95
	L= 1 H= 14			
1	21*	17	14-	10
2	21*	14	9-	10-
3	57	64	33-	55-
4	19*	18	16	9
5	45	65	65	7-
6	23	29	3-	29-
7	14*	6	5	3-
	L= 1 H= 15			
1	15*	26	24	8-
2	24	34	34	6
3	37	39	39	3
	L= 2 H= 1			
0	851	868	0	868-
	L= 2 H= 2			
0	1532	1573	1573	0
	L= 2 H= 3			
0	401	431	0	431
	L= 2 H= 4			
0	722	745	745	0
	L= 2 H= 5			
0	16*	12	0	12-
	L= 2 H= 6			
0	120	121	121	0
	L= 2 H= 7			
0	126	114	0	114
	L= 2 H= 8			
0	235	237	237	0
	L= 2 H= 9			
0	153	140	0	140
	L= 2 H= 10			
0	46	53	53-	0
	L= 2 H= 11			
0	58	63	0	63
	L= 2 H= 12			
0	23*	3	3	0
	L= 2 H= 13			
0	36	24	0	24-
	L= 2 H= 14			
0	21	17	17-	0
	L= 2 H= 0			
1	1265	1283	1283-	0
2	538	582	582-	0
3	407	416	416	0
4	302	296	296	0
5	163	161	161	0
6	568	559	559	0
7	109	98	98	0
8	235	207	207-	0
9	168	148	148-	0
10	237	221	221	0
11	40	33	33	0
12	292	286	286	0
13	165	148	148	0
14	143	133	133	0
15	132	112	112-	0
16	31	20	20	0
17	20*	22	22	0
18	34	29	29-	0
	L= 2 H= 1			
1	899	916	295-	868-
2	715	751	208	721-
3	250	254	233-	100-
4	181	177	94-	150-
5	533	499	170-	469
6	751	689	444-	527-
7	345	316	67-	308-
8	154	132	116-	63-
9	84	66	66-	1-
10	189	170	88	146-
11	105	97	10-	93-
12	45	48	48-	4
13	65	63	57	26-
14	161	143	19-	142-
15	176	140	5	140-
16	91	66	36-	59-
17	34	36	9	28-
18	64	58	58	10-
	L= 2 H= 2			
1	1141	1061	369*	994-
2	472	490	442-	212
3	74	82	71-	41
4	78	70	65	26
5	292	312	152	273-
6	472	466	409	224
7	122	108	100-	43-
8	69	57	18-	54
9	206	174	160-	68-
10	127	104	20	102
11	152	135	117	66
12	152	124	114-	48
13	39	33	28-	17-
14	136	133	133	7
15	102	81	53-	61-
16	22*	9	9-	2-
17	19*	14	11	9
18	35	35	35-	5
	L= 2 H= 3			
1	669	674	24	674-
2	323	352	351-	24-
3	195	199	192-	52
4	285	322	317	54-
5	242	250	192-	161
6	202	188	13	188-
7	419	426	165-	392-
8	140	123	55-	110-
9	161	152	168-	107
10	141	134	43-	127-
11	261	258	248-	72-
12	253	224	80	209-
13	81	79	77-	16
14	151	112	56	97-
15	172	143	97-	106-
16	94	85	84-	10-
17	18*	36	35-	7
18	44	38	24-	30-
	L= 2 H= 4			
1	257	264	7-	264-
2	221	228	223-	45-
3	72	75	42	62-
4	105	101	67-	74-
5	279	306	292	229-
6	244	260	215	147
7	171	173	44	167-
8	236	227	226-	12
9	118	113	34	108-
10	43	35	22-	27
11	325	306	147	269-
12	43	48	47-	13-
13	49	50	47-	17-
14	163	169	102	135
15	83	74	14-	73-
16	51	55	28-	47
17	17*	12	1	12-
18	13*	15	14-	6
	L= 2 H= 5			
1	513	555	220-	509-
2	224	215	212-	35
3	136	128	107-	71
4	349	359	334	132
5	349	373	150-	341
6	74	76	64-	41
7	230	218	133-	172-
8	144	138	125-	58
9	94	88	74-	44-
10	38	38	35	14
11	134	131	49-	122
12	88	101	24	98
13	175	186	129-	134
14	80	88	33	82
15	93	80	24-	75-
16	107	95	90-	30
17	57	54	54-	0
	L= 2 H= 6			
1	354	367	244-	274-
2	260	261	216-	146
3	243	235	72	224
4	198	203	203-	4-
5	318	348	14-	348-
6	249	267	48	262-
7	160	154	95-	122-
8	177	180	92-	155
9	148	148	10	148-
10	24*	8	4	7-
11	110	106	17-	104-
12	24*	23	23	1-
13	63	62	41	46-
14	22*	27	27-	0
15	71	72	24-	68-
16	70	77	49-	60
17	76	78	48	61
	L= 2 H= 7			
1	205	192	160-	106-
2	273	276	149-	232
3	98	95	69	65
4	271	270	253	94
5	198	198	7-	198
6	222	226	185-	129
7	162	158	145-	119-
8	258	262	26	261
9	34	14	4	14
10	85	82	44	68
11	116	130	55	118
12	116	132	65-	115
13	75	82	58-	58
14	33	30	7-	29
15	18*	13	3-	13-
16	62	63	44-	46
	L= 2 H= 8			
1	218	221	142-	169-
2	254	264	206-	166
3	191	180	59	170
4	176	182	181-	22-
5	245	243	29	241-
6	58	63	43	47
7	59	52	51-	10
8	140	152	31	149
9	49	51	13	49
10	37	39	38-	10
11	41	45	37	26-
12	68	83	69-	46-
13	30	26	24	7
14	19*	12	1-	12-
15	66	74	38-	63-
16	67	87	82-	26
	L= 2 H= 9			
1	108	97	38	89-
2	335	313	299-	93
3	197	168	144	86
4	327	309	216	221
5	77	70	15-	68
6	82	76	35	67
7	25*	29	17	24-
8	76	79	8	79
9	68	70	63	31
10	70	66	6-	66
11	32	39	19	33
12	66	73	29	67
13	26	22	5	22
14	58	54	37	39
15	20	29	5	28-
	L= 2 H= 10			
1	81	87	85-	17-
2	89	94	50-	79
3	204	181	16-	180
4	165	142	1-	142-
5	89	88	47	75-
6	35	37	13-	34-
7	57	66	25	62
8	98	103	92-	48-
9	115	130	69-	110
10	34	34	32-	12-
11	20*	24	23	5
12	54	50	17	47-
13	15*	8	7	4
14	11*	11	4-	10-
	L= 2 H= 11			
1	23*	24	13-	20-
2	28	33	29	16
3	192	198	1-	198
4	23	37	14-	31-
5	31	43	9-	32-
6	34	48	17-	45-
7	32	31	30-	10
8	19	15	2	15
9	67	64	11-	63
10	63	63	59-	22-
11	47	54	52-	53
	L= 2 H= 12			
1	26	31	29	12
2	120	114	113-	14-
3	46	60	13	59-
4	124	122	103	64-
5	35	38	34	17-
6	18*	17	17-	2-
7	16*	16	16	0
8	15*	18	6-	17
9	60	70	63	32-
	L= 2 H= 14			
1	17*	8	1-	7
2	17*	21	16	13
3	119	124	22	122
4	15*	6	6	2-
5	14*	14	10-	10-
	L= 3 H= 1			
0	327	335	0	335-
	L= 3 H= 2			
0	214	244	244-	0
	L= 3 H= 3			
0	104	100	0	100-
	L= 3 H= 4			
0	531	517	517-	0
	L= 3 H= 5			
0	67	66	0	66
	L= 3 H= 6			
0	333	314	314-	0
	L= 3 H= 7			
0	30*	10	0	10-
	L= 3 H= 8			
0	46	37	37-	0
	L= 3 H= 9			
0	34*	1	0	1
	L= 3 H= 10			
0	81	82	82	0
	L= 3 H= 11			
0	35*	10	0	10
	L= 3 H= 12			
0	40	45	45	0
	L= 3 H= 13			
0	28*	4	0	4-
	L= 3 H= 14			
-0	22*	24	24	0
	L= 3 H= 0			
1	219	203	0	203-
2	258	229	0	229
3	327	303	0	303-
4	179	156	0	156-
5	156	131	0	131-
6	444	405	0	405
7	626	586	0	586-
8	285	252	0	252-
9	54	45	0	45-
10	36	34	0	34
11	148	136	0	136-
12	58	26	0	26
13	193	202	0	202-
14	231	218	0	218-
15	67	58	0	58-
16	30*	18	0	18
17	69	62	0	62-
18	41	42	0	42-
	L= 3 H= 1			
1	163	174	173	21
2	317	325	256-	199-
3	110	100	86-	49-
4	124	107	15	106
5	290	265	265-	2-
6	359	326	283	161-
7	388	369	364	62-
8	232	209	205-	42-
9	259	227	224-	40-
10	94	82	74-	34
11	125	130	125-	35-
12	96	93	0	93
13	186	186	184	30-
14	213	184	184-	13-
15	188	169	147-	22-
16	58	52	46-	24
17	26*	25	14	20
18	35	40	4	40
	L= 3 H= 2			
1	494	503	446-	233-
2	256	253	245-	12
3	69	66	62-	23
4	212	219	12	218-
5	302	296	82-	285-
6	204	208	201-	56
7	251	245	19	244-
8	193	185	103-	183-
9	138	128	126-	22-
10	144	144	138-	44-
11	34*	22	5-	21
12	175	179	142-	110
13	368	298	126	269-
14	301	282	130-	251-
	L= 3 H= 3			
15	33*	35	17-	30-
16	87	79	51-	60
17	58	50	50	4-
18	58	63	62-	5
	L= 3 H= 4			
1	150	146	127-	72
2	170	171	156-	69-
3	192	202	162-	120-
4	108	113	72-	87
5	213	220	190-	109
6	130	134	35	129-
7	398	388	372	110
8	229	205	146-	144-
9	241	215	173-	127
10	117	116	65	96
11	138	129	46-	121-
12	99	96	36	90-
13	306	336	336	7-
14	128	104	21	102-
15	116	116	104-	52
16	28*	30	9-	28
17	24*	8	3-	8
18	44	51	47	18-
	L= 3 H= 5			
1	340	349	278	212-
2	526	579	574-	81-
3	218	221	130-	179
4	255	257	182-	181-
5	91	87	86	10-
6	432	445	286-	340
7	67	49	40	29-
8	331	331	178-	280-
9	157	156	154-	22
10	167	163	144-	75
11	247	253	216	132
12	165	171	87-	147
13	116	127	97-	82-
14	105	96	15-	95-
15	53	57	41-	40
16	23	41	17-	37
17	22*	33	30	12-
	L= 3 H= 6			
1	364	345	338	65
2	345	357	61-	352-
3	144	149	149-	12
4	77	82	44-	70
5	173	184	148-	109-
6	127	130	54	118-
7	294	348	339	76
8	292	295	211-	206-
9	177	185	107-	151
10	208	193	71	179
11	195	200	198-	28-
12	188	184	111	147-
13	163	156	155	22
14	32*	8	5-	6-
15	116	118	107-	50
16	33	56	15-	54
17	35	36	25	29
	L= 3 H= 7			
1	145	146	135	56
2	102	106	27-	103-
3	142	142	71-	123
4	119	105	85-	61-
5	263	267	171	206
6	300	321	210-	243
7	201	209	208	24
8	238	250	154-	197-
9	168	177	154-	87
10	83	85	75-	39
11	134	141	118	78
12	124	131	105-	79
13	66	85	85-	1-
14	142	135	132-	28-
15	137	137	19-	136
16	47	43	24	36
	L= 3 H= 8			
1	79	67	48	47
2	156	167	98	134-
3	71	65	53-	38-
4	88	86	79	32
5	158	155	21	153-
6	225	221	209	73-
7	174	186	152	65-
8	171	182	67-	170-
9	157	167	147-	2-
10	115	117	75	90
11	46	46	1-	46-
12	117	119	65	99-
13	122	112	112	6
14	34	40	17-	36-
15	38	50	42-	29
16	49	53	3-	53
	L= 3 H= 9			
1	159	153	79	131
2	52	34	34	4
3	211	206	65-	195
4	143	158	96	126
5	187	196	74-	181
6	111	99	94-	29
7	79	81	77-	24
8	66	63	50-	39
9	136	128	90-	91
10	85	79	65	55
11	114	130	99	84
12	62	61	34-	51
13	49	45	43-	13-
14	90	82	73-	38-
15	88	92	30-	87
	L= 3 H= 9			
1	113	95	35	88
2	60	60	38	46-
3	123	124	100-	73
4	30	41	30	28
5	56	47	29	37-
6	51	51	27	44-
7	50	54	53	5
8	58	63	4-	63-
9	76	83	11-	83
10	96	101	26	98
11	87	94	4	94-
12	101	100	44	90-
13	37	41	41	6-
14	30	39	6-	39-
	L= 3 H= 10			
1	96	47	37	30
2	31	12	8	10-
3	117	109	81-	73
4	98	96	95	13
5	96	97	63	74
6	39	44	1	44
7	57	51	41	30
8	66	69	69	5-
9	97	99	86-	48
10	138	149	138	55
11	138	137	123	60
12	24*	16	11	11
13	34	42	19-	37
	L= 3 H= 11			
1	72	66	1-	64
2	78	84	42-	73-
3	86	91	41-	81
4	163	162	37-	158
5	41	46	8-	45-
6	52	48	22	43-
7	35	38	30	23-
8	88	82	35-	75-
9	81	78	49-	61
10	130	134	5	134
11	51	52	19	49-
12	47	52	14	50-
	L= 3 H= 12			
1	32*	21	1	21
2	82	83	82	12-
3	76	68	57-	36-
4	107	118	118	6-
5	86	60	77	22-
6	35	20	11	16-
7	33	38	32	21
8	66	60	50	33-
9	104	107	105-	22
10	82	101	91	43
	L= 3 H= 13			
1	28*	39	35	18
2	28*	21	8	19

Table 7. Continued

3		49	34-	35-	16	20*	21	20-	6	11	46	44	1-	44-			L= 5 H= 3				2	67	58	47	34-
4	96	98	41-	89	17	42	45	19-	41-	12	27	40	15-	37-	1	145	153	7-	153		3	24*	25	18	17
5	39	41	32	26-			L= 4 H= 4					L= 4 H= 11			2	152	157	154-	34		4	140	122	110	52
6	31	27	18	20-	1	366	335	256-	217-	1	27	28	25	13-	3	104	114	11	113		5	114	96	32	90
7	21*	17	14-	9-	2	332	358	296-	201	2	105	105	105-	10	4	264	264	30	262		6	48	42	27-	32
8	23	32	1	32-	3	251	254	1	254	3	189	161	153	49	5	202	216	193-	97-		7	54	44	44	4-
	L= 3 H= 14				4	28	19	19-	1	4	150	124	124	4	6	157	171	131	109		8	62	57	34-	47-
1	22*	18	1	18-	5	169	172	111	131-	5	62	56	56	4-	7	162	168	166	26		9	70	66	55-	36
2	56	65	51	40-	6	278	294	215	201-	6	61	54	52-	14	8	296	306	294-	86		10	58	56	52	20
3	36	35	16-	32-	7	96	94	89-	30	7	31	19	11-	15-	9	96	95	37-	88		11	33	44	41	14
4	74	82	65	51	8	161	157	89-	130	8	76	65	24-	60	10	113	114	21-	113				L= 5 H= 11		
5	30	36	32	17-	9	110	112	14-	111	9	115	109	107	15	11	89	98	90-	39		1	35	30	22	20
	L= 4 H= 1				10	90	90	89	8	10	26	16	6-	15	12	137	137	126	55		2	77	79	51	60-
0	284	255	0	255-	11	147	155	1-	155			L= 4 H= 12			13	125	118	115	29		3	68	66	64-	15
	L= 4 H= 2				12	58	59	57-	14	1	91	70	8-	70-	14	101	186	169-	78		4	39	40	23-	33-
0	225	251	251	0	13	133	129	57	116	2	93	86	35-	79	15	145	148	134-	64		5	139	119	25	116-
	L= 4 H= 3				14	124	92	88	29-	3	82	71	9-	70	16	62	65	23-	61		6	77	70	37	60-
0	654	687	0	687-	15	74	69	53-	44-	4	80	76	45-	62-			L= 5 H= 4				7	18*	13	5	12-
	L= 4 H= 4				16	42	36	29-	22	5	98	89	17-	88-	1	70	71	57-	42-		8	78	71	17-	69-
0	346	381	381	0	17	82	95	4	95	6	21*	11	5-	10	2	92	94	20-	92		9	48	60	13-	58
	L= 4 H= 5						L= 4 H= 5			7	19*	17	4-	17	3	25	33	12-	31				L= 5 H= 12		
0	157	151	0	151-	1	315	366	220-	290-	8	33	38	19	33	4	60	59	43-	41-		1	35	36	28	22
	L= 4 H= 6				2	299	330	280-	175	9	14*	9	4	8-	5	81	87	25-	84		2	49	49	21	45-
0	238	241	241	0	3	85	82	65-	51			L= 4 H= 13			6	335	350	211-	280		3	26	27	27-	4-
	L= 4 H= 7				4	126	131	86	99	1	17	9	8	5	7	262	280	112	257-		4	120	117	104	53
0	25*	12	0	12-	5	196	211	196-	78	2	84	83	82-	14-	8	214	214	107-	185-		5	54	52	18	49
	L= 4 H= 8				6	233	263	241-	105-	3	156	158	158	5-	9	155	148	126-	78		6	15*	9	4	7
0	33	5	5-	0	7	337	362	321-	167-	4	88	88	87	11	10	83	82	42	71		7	12*	25	22	13-
	L= 4 H= 9				8	126	115	9-	114	5	44	53	11	52	11	30	36	23	27				L= 5 H= 13		
0	28*	11	0	11	9	129	136	126-	51	6	15*	12	6-	11-	12	174	161	160-	20		1	28	31	5-	30
	L= 4 H= 10				10	150	151	27-	149			L= 4 H= 14			13	115	114	20-	112-		2	73	89	18	87-
0	60	60	60	0	11	146	140	137-	30-	1	28	42	6-	42-	14	189	192	143-	127-		3	84	93	78-	50
	L= 4 H= 11				12	135	112	103-	44-	2	43	59	9	58	15	51	49	33-	36				L= 6 H= 1		
0	30	31	0	31-	13	162	153	150-	30-			L= 5 H= 1			16	18	26	23-	12		0	377	417	0	417-
	L= 4 H= 12				14	105	93	57	73-	0	92	138	0	138			L= 5 H= 5						L= 6 H= 2		
0	21	20	20-	0	15	91	88	64-	61-			L= 5 H= 2			1	22	22	6-	21		0	73	90	90	0
	L= 4 H= 13				16	67	74	34-	66	0	297	301	301-	0	2	201	217	182-	117				L= 6 H= 3		
0	23	23	0	23-			L= 4 H= 6					L= 5 H= 3			3	118	115	90	71		0	233	278	0	278-
	L= 4 H= 14				1	89	89	89-	8	0	356	360	0	360	4	202	214	93	193				L= 6 H= 4		
0	29	36	36-	0	2	58	56	56-	5			L= 5 H= 4			5	102	111	36	105-		0	167	189	189	0
	L= 4 H= 0				3	187	177	35-	174	0	32	41	41-	0	6	316	320	285	144				L= 6 H= 5		
1	19	21	21-	0	4	105	95	27-	91-			L= 5 H= 5			7	122	124	114	49-		0	203	225	0	225-
2	148	145	145-	0	5	223	249	126	214-	0	247	263	0	263	8	77	67	66-	8				L= 6 H= 6		
3	119	112	112-	0	6	224	249	225	106			L= 5 H= 6			9	62	56	25-	50		0	172	183	183	0
4	346	384	384-	0	7	205	216	22-	215	0	169	189	189-	0	10	119	124	8-	123				L= 6 H= 7		
5	52	45	45-	0	8	62	54	18	51			L= 5 H= 7			11	103	81	28	76		0	121	128	0	128-
6	148	149	149	0	9	45	43	8-	42	0	111	129	0	129	12	132	116	116	6				L= 6 H= 8		
7	289	290	290-	0	10	49	42	22-	36-			L= 5 H= 8			13	143	151	144	41		0	169	173	173	0
8	208	192	192-	0	11	98	98	90	38-	0	77	66	66-	0	14	85	62	61-	9				L= 6 H= 9		
9	157	154	154-	0	12	27	36	24	27-			L= 5 H= 9			15	89	92	76-	52		0	56	63	0	63-
10	45	49	49	0	13	51	50	42	26	0	39	31	0	31			L= 5 H= 6						L= 6 H= 10		
11	30*	13	13	0	14	129	124	108	62			L= 5 H= 10			1	160	160	160	11		0	58	60	60	0
12	74	74	74-	0	15	51	50	26	42-	0	55	62	62-	0	2	184	199	191-	56-				L= 6 H= 11		
13	152	155	155-	0	16	13*	10	3	10			L= 5 H= 11			3	185	193	137-	136		0	22*	0	0	9-
14	29*	0	0	0			L= 4 H= 7			0	22*	4	0	4	4	35	41	32-	26-				L= 6 H= 12		
15	74	73	73-	0	1	232	259	141-	218-			L= 5 H= 12			5	106	94	55-	77		0	17*	13	13-	0
16	22*	16	16-	0	2	200	188	142-	123	0	29	12	12-	0	6	124	133	131-	19-				L= 6 H= 0		
17	31	31	31-	0	3	34	30	23	19-			L= 5 H= 13			7	124	123	52-	112-		1	161	173	173-	0
	L= 4 H= 1				4	331	325	203	254	0	21	5	0	5	8	178	168	100-	135-		2	283	331	331-	0
1	482	489	202-	446-	5	215	226	173-	145			L= 5 H= 0			9	155	179	130-	124		3	36	46	46-	0
2	147	154	151-	31-	6	65	64	36-	52-	1	352	369	0	369-	10	61	57	56	14		4	118	119	119-	0
3	284	292	89-	278	7	120	115	105-	47	2	125	143	0	143-	11	191	174	140	104		5	165	181	181	0
4	150	148	137	57	8	32	19	7	18	3	25	18	0	18-	12	72	54	49-	22		6	87	85	85	0
5	95	84	83-	18-	9	32	37	28-	25-	4	93	90	0	90-	13	94	83	61-	57-		7	91	98	98-	0
6	455	447	231	383-	10	107	108	60	90	5	70	59	0	59-	14	65	61	4-	61-		8	193	227	227-	0
7	266	270	79-	258-	11	60	60	42-	43	6	43	5	0	5	15	23	27	21-	18-		9	31*	7	7	0
8	124	123	34	119-	12	40	49	14-	47	7	166	162	0	162-			L= 5 H= 7				10	29	10	10-	0
9	51	57	30	48	13	87	82	81-	6	8	126	130	0	130-	1	175	178	152	91		11	42	46	46	0
10	74	76	54-	53-	14	64	64	49	42	9	26*	13	0	13-	2	160	157	116-	106-		12	141	153	153-	0
11	44	58	38-	43	15	36	38	8-	37-	10	27*	24	0	24-	3	88	84	30-	79		13	25*	17	17	0
12	182	179	45	173-			L= 4 H= 8			11	27*	20	0	20	4	75	74	1	74		14	22*	7	7	0
13	58	57	57-	8	1	144	150	123-	86-	12	174	206	0	206	5	43	45	35	28-		15	56	66	66-	0
14	122	126	36-	120-	2	185	111	67	89	13	89	91	0	91-	6	75	71	41	58				L= 6 H= 1		
15	96	89	71-	54-	3	146	140	73	119	14	83	78	0	78-	7	151	127	99	78		1	297	332	99	317-
16	27	31	25-	18	4	124	113	18	111-	15	17	26	0	26	8	101	82	79-	22-		2	68	77	23	74
17	18*	2	0	2	5	131	124	60	109-	16	105	111	0	111	9	146	133	63	118		3	128	127	55	115
	L= 4 H= 2				6	111	112	91	66-			L= 5 H= 1			10	178	165	41	160		4	25	22	2-	22-
1	489	525	348-	393	7	53	54	48	23	1	166	178	71-	163	11	62	51	13-	49-		5	133	126	31	122
2	178	188	166-	89	8	44	46	45-	8-	2	111	121	121-	4	12	90	84	74	39-		6	204	194	111-	159-
3	200	206	159	130	9	58	64	52	38-	3	93	97	14	96	13	59	62	61	4-		7	90	78	72-	32
4	121	121	74-	96-	10	32	35	14-	32-	4	99	100	80	60	14	38	48	32-	36		8	52	54	45	29-
5	82	69	50	47	11	68	58	6	58-	5	200	196	165-	106-			L= 5 H= 8				9	129	133	53-	122
6	171	170	154	72	12	67	61	60	12-	6	94	98	52	83	1	88	78	44	64		10	64	72	10	71
7	74	62	38-	50-	13	64	63	61	14	7	75	77	72	26	2	95	93	6-	93-		11	53	53	21-	59-
8	277	278	277-	10	14	16*	24	23	6-	8	246	247	237-	67	3	121	118	116-	20		12	59	69	31-	62-
9	132	121	47-	111			L= 4 H= 9			9	185	198	184-	74	4	28	29	7-	28-		13	100	94	75-	56
10	119	111	108	28	1	151	140	91-	106-	10	83	83	20	80	5	56	58	52	26		14	78	79	27	74-
11	108	105	17-	103-	2	182	178	33-	171	11	117	127	117-	48	6	73	68	62-	27		15	18*	32	29	13
12	87	96	68-	67-	3	140	130	129	17-	12	83	97	95	17	7	104	94	72	61				L= 6 H= 2		
13	28*	16	1-	16-	4	131	135	125	34	13	93	84	85	17-	8	143	118	10-	118-		1	137	148	148-	1-
14	59	61	28-	55	5	28*	16	12	10	14	123	117	100-	60	9	195	171	147-	89		2	180	198	197-	9
15	122	111	108-	25-	6	101	90	90-	10	15	128	135	130-	37	10	32	31	5-	31		3	188	190	98-	163
16	54	62	58-	20	7	41	44	27-	35-	16	46	50	38-	33	11	95	93	62	69		4	132	143	137-	41
17	21	35	25-	25	8	121	114	26-	110			L= 5 H= 2			12	77	70	65-	25		5	232	236	208	112
	L= 4 H= 3				9	71	67	55	37-	1	137	159	118	107-	13	48	46	45-	3		6	217	205	129	159-
1	737	758	503-	567-	10	42	39	33	20	2	24	25	19-	16			L= 5 H= 9				7	164	172	139-	101
2	173	166	164-	25	11	83	77	59	56	3	59	63	52	35-	1	51	50	35	35		8	230	233	175-	154
3	209	209	175-	115	12	38	45	29-	34	4	167	172	130-	112-	2	127	127	30-	123-		9	55	56	28-	48
4	231	243	151	190	13	16*	24	22-	9	5	26	17	17-	2	3	35	39	4	39-		10	38	50	48-	16-
5	370	401	249-	315			L= 4 H= 10			6	377	400	164-	365	4	33	27	3-	27		11	44	48	27	40
6	248	262	1-	262-	1	131	121	7-	121-	7	178	186	14	185-	5	84	68	12	67-		12	56	69	50-	48
7	269	287	257-	127-	2	84	72	10	71	8	212	222	96-	201-	6	104	95	80	51-		13	131	134	14	133
8	59	58	57	5-	3	128	124	24	120	9	70	74	74-	10-	7	100	79	73	32		14	37	54	24	48
9	94	85	85-	4-	4	39	44	18-	40-	10	107	107	18-	105	8	92	78	20-	75-		15	34	49	45-	21
10	68	65	20-	61	5	89	89	3	89-	11	69	78	60	49-	9	56	52	48-	18				L= 6 H= 3		
11	28*	11	2-	11-	6	42	44	43	12-	12	88	100	34	94	10	62	60	36	47		1	75	83	28-	78-
12	68	71	41-	58	7	75	65	11-	64-	13	180	170	87-	146-	11	85	79	42	67-		2	90	98	45	87
13	177	153	119-	95	8	90	83	14-	81	14	114	102	67-	77-	12	59	71	50	50-		3	122	119	89	80
14	120	104	32-	94-	9	92	90	85	29-	15	52	49	34-	35			L= 5 H= 10				4	54	69	64	25-
15	97	85	67-	53-	10	54	47	17-	44-	16	45	53	14	52	1	86	85	18	83		5	159	157	13	157-

Table 7. Continued

6	263	271	176-	207-	3	121	126	59	112			L= 7 H= 1			8	73	64	45	46-	11	16*	13	3	12-
7	204	191	92-	167-	4	77	72	66	28	0	150	157	0	157	9	139	119	5	119			L= 7 H= 7		
8	28*	5	0	5-	5	59	56	28-	49-			L= 7 H= 2			10	89	64	64	6	1	43	39	36	13
9	104	100	10-	99	6	113	92	90-	16-	C	15*	10	10-	0	11	94	78	56	54	2	40	47	44-	18-
10	53	53	42	32	7	144	122	70-	100-			L= 7 H= 3			12	76	60	18-	57	3	120	125	120	32
11	28*	28	9	27-	8	61	56	6	56	0	117	151	0	151	13	88	87	0	87-	4	39	49	19	45
12	64	64	17-	62-	9	62	54	52	12			L= 7 H= 4					L= 7 H= 3			5	60	69	44	54-
13	58	55	32-	45-	10	78	62	13-	61	U	98	119	119-	0	1	38	48	40-	26-	6	49	56	45	34
14	49	52	39	34-	11	34	31	24-	20-			L= 7 H= 5			2	44	50	47-	16-	7	115	108	107	14
15	24	36	23	27	12	98	80	79-	12-	C	160	189	0	189	3	44	43	26	34	8	66	66	56-	35-
		L= 6 H= 4			13	30	41	38-	14-			L= 7 H= 6			4	66	51	45	24	9	44	56	6-	55
1	289	304	224-	207			L= 6 H= 8			U	23*	31	31	0	5	67	69	55-	42-	10	41	51	23-	46
2	91	86	38-	77	1	38	24	24-	6-			L= 7 H= 7			6	218	210	173	119			L= 7 H= 8		
3	188	191	27	189	2	81	80	60	52	0	107	115	0	115	7	84	86	33-	80	1	96	90	86	25-
4	82	79	14-	78-	3	138	129	48-	120			L= 7 H= 8			8	65	50	25-	44	2	39	43	33-	27-
5	136	120	117	28	4	69	64	12-	63-	C	112	116	116-	0	9	107	80	72-	35	3	97	86	21-	83
6	146	147	88	119	5	156	123	67	102-			L= 7 H= 9			10	116	99*	7	99	4	75	74	66	34
7	299	313	116-	291	6	159	134	131	27-	0	39	54	0	54	11	41	46	46-	5	5	76	84	4-	84
8	106	105	69-	79	7	83	76	69-	33			L= 7 H= 10			12	87	85	82	22	6	94	96	72-	63
9	71	74	27-	69	8	194	87	53	70	C	67	67	67-	0	13	15*	8	6-	5	7	112	117	39	111-
10	34	41	27	31	9	24*	9	5-	8			L= 7 H= 11					L= 7 H= 4			8	63	69	57-	39-
11	30	30	6	29-	10	50	38	14	35-	C	30	35	0	35	1	111	136	121	62-	9	51	50	46-	21
12	25*	10	1-	10-	11	45	44	41	15-			L= 7 H= 0			2	77	84	82	16-			L= 7 H= 9		
13	84	80	37	71	12	47	61	48	38-	1	39	60	0	60-	3	40	29	27-	10	1	99	109	93	56
14	72	71	19-	68			L= 6 H= 9			2	108	126	0	126	4	107	114	85	76-	2	77	87	18	85-
		L= 6 H= 5			1	31	39	28-	27-	3	94	82	0	82	5	68	64	4	63	3	64	81	11-	80
-1	195	196	154-	120-	2	134	112	95-	60	4	121	111	0	111-	6	84	77	53	57-	4	19*	27	2	27
2	141	146	10-	146	3	86	72	71	12-	5	127	93	0	93-	7	189	186	60	176-	5	98	114	77	84-
3	116	117	100	61	4	125	100	73	67	6	233	213	0	213	8	71	62	39-	49-	6	64	66	62	22
4	214	213	152	149	5	52	44	36-	26	7	150	123	0	123-	9	130	110	8	110	7	57	72	72	0
5	109	107	83-	67	6	97	71	69-	14	8	179	162	0	162-	10	21*	27	26	9	8	56	81	46-	66-
6	136	143	44-	136-	7	109	90	90-	11-	9	120	104	0	104	11	91	74	72	14-			L= 7 H= 10		
7	29*	25	13	21-	8	57	48	21	43	10	96	72	0	72	12	34	36	30	20	1	52	63	61	14
8	62	57	47	33-	9	59	56	25	50-	11	107	92	0	92	13	68	87	6-	87-	2	49	60	6	60-
9	58	64	48	42	10	42	47	5	47	12	56	42	0	42			L= 7 H= 5			3	69	77	75-	19
10	33	35	31	17-			L= 6 H= 10			13	141	136	0	136-	1	38	52	7	52	4	39	51	11-	50
11	45	53	43	32-	1	106	82	56-	61-			L= 7 H= 1			2	22*	4	4	0	5	25	50	33-	38
12	37	19	19-	4	2	109	95	22	93	1	191	198	178-	87-	3	73	79	78	12	6	32	57	53-	19-
13	36	40	5-	39	3	25*	5	0	5	2	134	157	157-	15	4	56	63	8-	63			L= 7 H= 11		
14	58	62	39	49-	4	104	90	47-	77-	3	57	67	53-	42-	5	23*	34	23-	25-	1	38	61	59	15
		L= 6 H= 6			5	162	139	7	139-	4	32	13	6	12	6	61	90	39-	81			L= 8 H=		
1	131	148	140-	47-	6	72	68	56	38-	5	277	261	258-	42	7	71	84	28	79	1	188	174	174-	0
2	194	180	28-	178	7	58	57	46-	33	6	162	100	86	51	8	142	127	124-	29	2	141	146	146-	0
3	238	228	52	222	8	76	72	62	36	7	86	72	26	67	9	93	85	9-	85	3	53*	37	37-	0
4	67	70	46	53-	9	27	26	17	20-	8	147	134	129-	37	10	78	72	9	72	4	52*	18	18-	0
5	132	133	128	34			L= 6 H= 11			9	104	84	82-	22-	11	18*	24	23	5-	5	229	249	249	0
6	88	86	82	25	1	74	70	58-	38-	10	42	24	8-	22	12	70	81	80	9	6	49*	65	65-	0
7	62	59	33-	49	2	124	115	47-	105	11	100	86	80-	31-			L= 7 H= 6			7	67	74	74-	0
8	81	74	17-	75	3	112	108	97	48-	12	85	76	67	34-	1	93	86	30	80-	8	141	141	141-	0
9	51	44	25	37	4	67	41	39	13	13	36	36	20	30	2	36	50	41	29			L= 9 H= 0		
10	128	125	116	45	5	80	78	63-	46			L= 7 H= 2			3	23*	2	2	0	1	61*	33	0	33
11	89	82	30	77	6	49	46	45-	8	1	76	126	76	101-	4	95	104	97	38-	2	74	64	0	64
12	53	45	44	4	7	34	29	21-	21	2	33	41	35	21	5	33	21	16	14	3	119	130	0	130
13	102	108	35	102			L= 6 H= 12			3	114	114	48-	103	6	79	93	52-	77	4	91	83	0	83-
14	13	29	27	11	1	71	73	32-	66-	4	62	59	44	39-	7	103	118	89	84-	6	51*	77	0	77
		L= 6 H= 7			2	69	74	7-	74	5	90	90	48-	76	8	59	56	17-	54-	7	110	119	0	119-
1	85	90	75-	50-	3	23	38	38	5-	6	130	113	59	98	9	45	54	45-	30	8	220	222	0	222
2	130	140	83-	113	4	61	82	16-	81-	7	265	260	60	253-	10	73	77	69	34					

An analysis of the thermal parameters of the S and C atoms, assuming the whole molecule as a rigid body, was carried out according to the method by Schomaker and Trueblood.[12] The rigid-body tensors arrived at are given in Table 5. The translational tensor **T** and the screw tensor **S** depend upon the origin, and they are in Table 5 given relative to the unique origin which symmetrizes **S**. This origin lies about 0.45 Å from the centre of gravity of the molecule, displaced along the three crystal axes by -0.41, -0.14 and 0.13 Å, respectively.

The r.m.s. difference between observed and calculated U_{ij}'s is 0.0050 Å^2. The maximum and minimum translation amplitudes are 0.228 and 0.204 Å, respectively, and the translational motion is thus not markedly anisotropic. The maximum and minimum libration amplitudes are 5.0 and 1.2°, 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 2,5-diphenyl-thiothiophthene molecule have also been carried out. The parts of the molecule treated in this way are, ring *A* plus C(5), ring *D* plus C(12), and the thiothiophthene system plus C(5) and C(12). The librational tensors from these calculations are listed in Table 6.

If one compares $\mathbf{L}_A$, $\mathbf{L}_{(C+B)}$, and $\mathbf{L}_D$ in Table 6 with **L** in Table 5, one notes that there are relatively small differences between the eigenvalues and eigenvectors of **L**, and the eigenvalues and eigenvectors of $\mathbf{L}_{(C+B)}$ and $\mathbf{L}_D$. $\mathbf{L}_A$, on the other hand, shows considerable deviations from **L**, $\mathbf{L}_{(C+B)}$, and $\mathbf{L}_D$. This indicates that the $(C+B+D)$ part of the molecule librates roughly as a rigid body, and that *A* has some additional libration relative to the $(C+B+D)$ part. The eigenvector of $\mathbf{L}_A$ corresponding to the largest libration, 9.1°, is directed roughly along C(5) – C(6) – C(9), which shows that the additional libration of *A* occurs about the C(5) – C(6) bond.

The rigid-body analyses 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 analyses of ring *A* plus C(5), the r.m.s. difference of U_{ij}'s is 0.0027 Å.[2] Similarly for rings *B* and *C* plus C(5) and C(12), and ring *D* plus C(12), the r.m.s. differences are 0.0032 and 0.0036 Å^2, respectively.

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

The average C–C bond length in the phenyl groups of the present structure is 1.387 Å from the *l* values in Table 1, 1.391 Å from the *l'* values, and 1.397 Å from the *l''* values. The latter average bond length is equal to the accepted length of the C–C bonds in benzene.

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