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The Crystal and Molecular Structure of 2-(*p*-Dimethylanilino)-4-phenyl-6a-thiathiophthene

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The crystal and molecular structure of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene has been determined from three-dimensional X-ray data. The compound crystallizes in space group $P2_1/c$, with unit cell dimensions $a = 7.158$ Å, $b = 7.413$ Å, $c = 33.237$ Å, and $\beta = 90.14°$. There are four molecules per unit cell.

The structure was solved by three-dimensional Patterson synthesis, and refined by the full-matrix least sqaures method. The refinement comprises 2378 reflections (Cu$K\alpha$) observed within $\theta = 71°$.

Equal S – S distances occur in the linear three sulphur sequence of the molecule, *i.e.* S(1) – S(6a) = 2.348 ± 0.0013 Å, S(6a) – S(6) = 2.350 ± 0.0013 Å with the angle S(1) – S(6a) – S(6) = 176.39 ± 0.05°. The other bond lengths in the 6a-thiathiophthene system are S(1) – C(2) = 1.705 ± 0.004 Å, S(6a) – C(3a) = 1.748 ± 0.003 Å, S(6) – C(5) = 1.689 ± 0.003 Å, C(2) – C(3) = 1.388 ± 0.004 Å, C(3) – C(3a) = 1.395 ± 0.004 Å, C(3a) – C(4) = 1.428 ± 0.004 Å, and C(4) – C(5) = 1.360 ± 0.004 Å.

The C(4) – C(14) bond to the phenyl group, and the C(2) – C(6) bond to the *p*-dimethylanilino group are 1.496 ± 0.004 Å and 1.455 ± 0.004 Å, respectively.

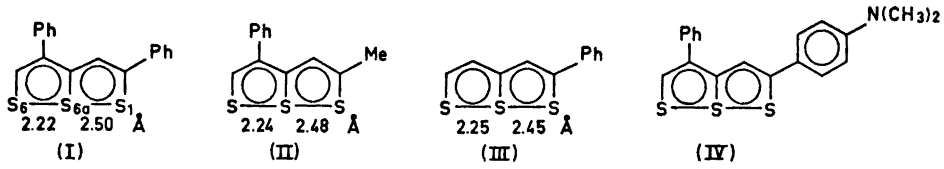
Both the 6a-thiathiophthene system and the *p*-dimethylanilino group are nearly planar. The phenyl group is twisted 81.8° about the C(4) – C(14) bond and the *p*-dimethylanilino group is twisted 12.7° about the C(2) – C(6) bond.

Other bond lengths in the *p*-dimethylanilino group are C(6) – C(7) = 1.410 Å, C(7) – C(8) = 1.372 Å, C(8) – C(9) = 1.413 Å, C(9) – C(10) = 1.418 Å, C(10) – C(11) = 1.370 Å, C(11) – C(6) = 1.407 Å, C(9) – N = 1.361 Å, N – C(13) = 1.458 Å, all ± 0.004 Å, and N – C(12) = 1.455 ± 0.005 Å.

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

In crystals of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene there are no intermolecular atomic distances shorter than corresponding van der Waals distances.

Unequal S – S bond lengths occur in the three-sulphur sequence of the compounds I – III.[1–3] In each of them S(1) – S(6a) is a longer bond than S(6a) – S(6), and one gets the idea that it is the substituent in 2-position which has perturbed the bonding in the sulphur sequence.



The present structure investigation of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene (IV) has been carried out in order to find the degree to which a *p*-dimethylanilino group in 2-position affects the sulphur-sulphur bonding in the 6a-thiathiophthene system.

STRUCTURE DETERMINATION

A brief account of the structure determination has been reported,[4] and a more detailed description is given here.

Crystals of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiopthene (IV) were generously supplied by Klingsberg.[5] The crystals are deep red and belong to the space group $P2_1/c$.

The structure analysis is based on X-ray data collected on a paper-tape controlled Siemens AED diffractometer using Cu$K\alpha$ radiation. 2378 reflections were observed within $\theta = 71°$.

Approximate coordinates for the sulphur atoms were found from a three-dimensional Patterson synthesis, and the remaining C and N atoms were found from a subsequent Fourier synthesis. The atomic parameters were refined by least squares methods, and the final R factor is 0.044.

A rigid-body analysis of the 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene molecule has been carried out according to the method of Schomaker and Trueblood,[6] and the S–S, S–C, C–C, and C–N bond lengths have been corrected for rigid-body libration according to Cruickshank's formula.[7] For further details with respect to the structure determination, see Experimental.

DISCUSSION

Molecular shape and dimensions. Bond lengths and angles in the 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene molecule, together with their standard deviations, are listed in Tables 1 and 2, and shown in Figs. 1a and 1b.

The equation for the least squares plane of the atoms of the 6a-thiathiophthene system, with weights inversely proportional to the respective standard deviations in coordinates is

$$0.65339\,X + 0.69964\,Y + 0.28747\,Z = 5.44667$$

with X, Y, and Z in Å units. Deviations from the plane for the atoms of the 6a-thiathiophthene system are S(1) −0.002, S(6a) −0.044, S(6) 0.051, C(2) 0.102, C(3) −0.045, C(4) −0.071, and C(5) −0.004 Å. One notes that C(2)

and C(4), to which the substituents are bonded, deviate most. Furthermore, the atoms C(6), C(9) and N lie 0.272, 0.651 and 0.865 Å, respectively, above the plane, and the atoms C(14) and C(17) lie 0.170 and 0.374 Å under it. Thus the almost linear sequences C(2)–C(6)–C(9)–N and C(4)–C(14)–

Table 1. Bond lengths (l) and standard deviation in bond lengths $\sigma(l)$ in 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene. Bond lengths (l') and (l'') with corrections for rigid-body libration are given for the S–S, S–C, N–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 group, the *p*-dimethylanilinogroup, and the thiathiophthene system are treated separately. For further explaination see the text.

Bond	l'' (Å)	l' (Å)	l (Å)	$\sigma(l)$ (Å)
S(1)–S(6a)	2.348	2.345	2.343	0.0013
S(6a)–S(6)	2.350	2.347	2.345	0.0013
S(1)–C(2)	1.705	1.707	1.702	0.004
S(6a)–C(3a)	1.748	1.751	1.744	0.003
S(6)–C(5)	1.689	1.691	1.685	0.003
C(2)–C(3)	1.388	1.386	1.384	0.004
C(3)–C(3a)	1.395	1.395	1.393	0.004
C(3a)–C(4)	1.428	1.426	1.424	0.004
C(4)–C(5)	1.360	1.361	1.359	0.004
C(2)–C(6)	1.455	1.455	1.453	0.004
C(6)–C(7)	1.410	1.403	1.400	0.004
C(7)–C(8)	1.372	1.372	1.370	0.004
C(8)–C(9)	1.413	1.408	1.403	0.004
C(9)–C(10)	1.418	1.411	1.408	0.004
C(10)–C(11)	1.370	1.370	1.368	0.004
C(11)–C(6)	1.407	1.402	1.397	0.004
C(9)–N	1.361	1.360	1.359	0.004
N–C(12)	1.455	1.449	1.444	0.005
N–(C13)	1.458	1.451	1.448	0.004
C(4)–C(14)	1.496	1.494	1.489	0.004
C(14)–C(15)	1.399	1.383	1.378	0.004
C(15)–C(16)	1.386	1.383	1.378	0.006
C(16)–C(17)	1.388	1.372	1.367	0.007
C(17)–C(18)	1.386	1.370	1.365	0.006
C(18)–C(19)	1.385	1.382	1.377	0.005
C(19)–C(14)	1.393	1.377	1.372	0.004

Bond	l (Å)	$\sigma(l)$ (Å)	Bond	l(Å)	$\sigma(l)$ (Å)
C(3)–H(3)	0.99	0.03	C(13)–H(131)	0.98	0.03
C(5)–H(5)	0.99	0.03	C(13)–H(132)	0.98	0.04
C(7)–H(7)	0.96	0.03	C(13)–H(133)	0.95	0.04
C(8)–H(8)	0.98	0.03	C(15)–H(15)	0.88	0.03
C(10)–H(10)	0.98	0.03	C(16)–H(16)	0.93	0.04
C(11)–H(11)	0.90	0.03	C(17)–H(17)	0.98	0.04
C(12)–H(121)	0.96	0.05	C(18)–H(18)	0.96	0.04
C(12)–H(122)	0.97	0.05	C(19)–H(19)	1.02	0.04
C(12)–H(123)	0.91	0.04			

Table 2. Bond angles ∠(ijk) in 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene. The standard deviations given in parentheses refer to the last digits of the respective values.

i	j	k	∠(ijk)°	i	j	k	∠(ijk)°
S(1)	S(6a)	S(6)	176.39(5)	C(19)	C(14)	C(4)	120.7(3)
C(2)	S(1)	S(6a)	94.3(1)	C(2)	C(3)	H(3)	123(1)
S(1)	S(6a)	C(3a)	88.8(1)	H(3)	C(3)	C(3a)	115(1)
C(3a)	S(6a)	S(6)	89.9(1)	C(4)	C(5)	H(5)	121(2)
S(6a)	S(6)	C(5)	91.9(1)	H(5)	C(5)	S(6)	118(2)
S(1)	C(2)	C(3)	115.4(2)	C(6)	C(7)	H(7)	119(2)
C(2)	C(3)	C(3a)	122.7(3)	H(7)	C(7)	C(8)	119(2)
C(3)	C(3a)	C(4)	123.2(2)	C(7)	C(8)	H(8)	120(2)
C(3a)	C(4)	C(5)	119.2(3)	H(8)	C(8)	C(9)	118(2)
C(4)	C(5)	S(6)	120.7(3)	C(9)	C(10)	H(10)	119(2)
C(3)	C(3a)	S(6a)	118.6(2)	H(10)	C(10)	C(11)	120(2)
C(4)	C(3a)	S(6a)	118.1(2)	C(10)	C(11)	H(11)	119(2)
S(1)	C(2)	C(6)	120.5(2)	H(11)	C(11)	C(6)	119(2)
C(3)	C(2)	C(6)	124.1(2)	C(14)	C(15)	H(15)	118(2)
C(2)	C(6)	C(7)	122.0(0)	H(15)	C(15)	C(16)	121(2)
C(6)	C(7)	C(8)	122.2(3)	C(15)	C(16)	H(16)	116(2)
C(7)	C(8)	C(9)	121.7(3)	H(16)	C(16)	C(17)	124(2)
C(8)	C(9)	C(10)	116.4(3)	C(16)	C(17)	H(17)	121(2)
C(9)	C(10)	C(11)	121.0(3)	H(17)	C(17)	C(18)	119(2)
C(10)	C(11)	C(6)	122.9(3)	C(17)	C(18)	H(18)	120(2)
C(11)	C(6)	C(7)	115.7(3)	H(18)	C(18)	C(19)	121(2)
C(11)	C(6)	C(2)	122.2(2)	C(18)	C(19)	H(19)	121(2)
C(8)	C(9)	N	121.8(3)	H(19)	C(19)	C(14)	118(2)
C(10)	C(9)	N	121.8(3)	N	C(12)	H(121)	111(3)
C(9)	N	C(12)	121.0(3)	N	C(12)	H(122)	110(3)
C(9)	N	C(13)	120.9(3)	N	C(12)	H(123)	110(2)
C(12)	N	C(13)	117.7(3)	N	C(13)	H(131)	109(2)
C(3a)	C(4)	C(14)	120.9(2)	N	C(13)	H(132)	111(2)
C(5)	C(4)	C(14)	119.9(3)	N	C(13)	H(133)	111(2)
C(4)	C(14)	C(15)	120.4(3)	H(121)	C(12)	H(122)	111(4)
C(14)	C(15)	C(16)	120.1(4)	H(122)	C(12)	H(123)	106(3)
C(15)	C(16)	C(17)	120.2(4)	H(123)	C(12)	H(121)	108(3)
C(16)	C(17)	C(18)	120.2(4)	H(131)	C(13)	H(132)	105(3)
C(17)	C(18)	C(19)	119.5(4)	H(132)	C(13)	H(133)	115(3)
C(18)	C(19)	C(14)	121.1(3)	H(133)	C(13)	H(131)	105(3)
C(19)	C(14)	C(15)	118.8(3)				

C(17) point in different directions relative to the plane of the 6a-thiathiophthene system.

The atoms of the dimethylamino group lie close to the least squares plane of the atoms of ring A. The equation for this plane is

$$0.43513\,X + 0.84609\,Y + 0.30680\,Z = 6.21719$$

and the deviations from the plane for N, C(12), and C(13) are 0.035, −0.041, and 0.005 Å, respectively.

The phenyl group D is twisted 81.8° about the C(4)−C(14) bond. This twist angle was taken as the angle between the normal to the plane through C(3a), C(4), C(5), and C(14), and the normal to the plane through C(4), C(14),

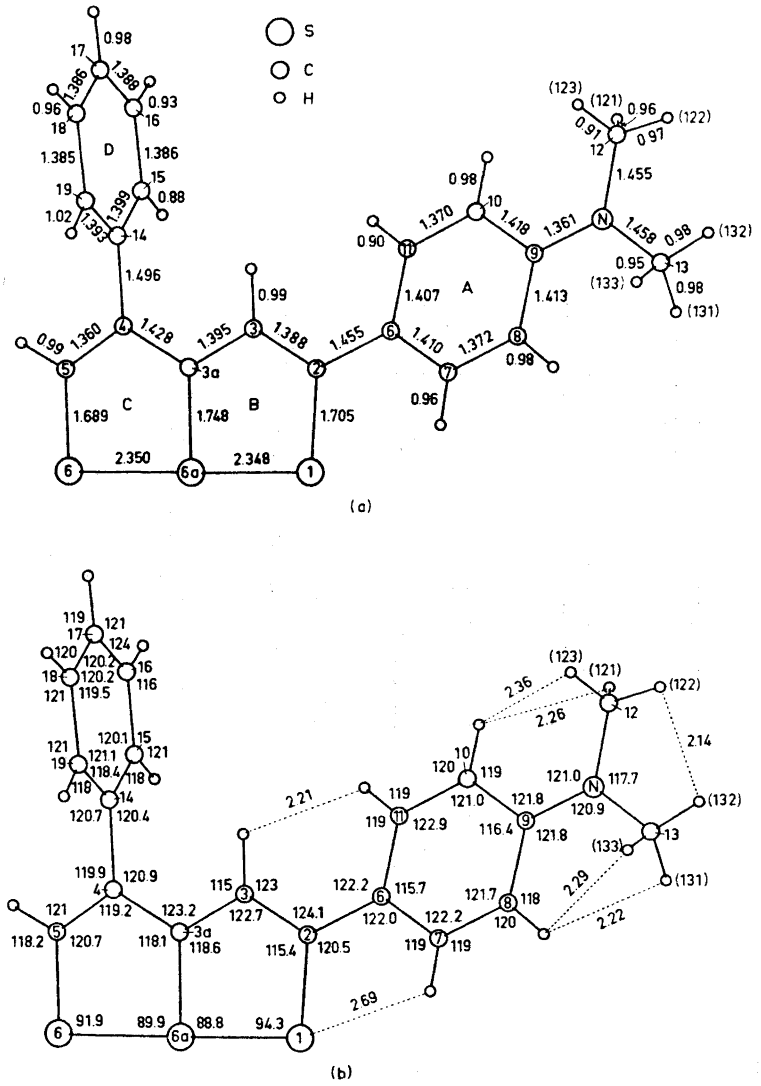


Fig. 1. (a) Bond lengths (Å) in the 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene molecule. (b) Bond angles (°) and intramolecular non-bonding distance (Å).

C(15), and C(19). Similarly, the twist angle of the *p*-dimethylanilino group about C(2)–C(6) is 12.7°.

It is seen from Fig. 1a that the *p*-dimethylanilino group has a quinoid structure. The lengths of the C(7)–C(8) and the C(10)–C(11) bonds, 1.372 and 1.370 ± 0.004 Å, are shorter than the accepted length, 1.397 Å, for the aromatic C–C bond in benzene, and the lengths of the other C–C bonds in

ring A, ranging from 1.407 to 1.418 ± 0.004 Å are longer. Furthermore, C(2)–C(6) = 1.455 ± 0.004 Å and C(9)–N = 1.361 ± 0.004 Å possess double bond character. The former bond is significantly shorter than the central C–C bond in diphenyl, 1.494 Å,[8] and the latter is almost as short as the aromatic C–N bond in pyridin, 1.340 Å.[9]

Comparison with related molecules. A comparison of bond lengths in 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene (IV) with bond lengths in 2,4-diphenyl-6a-thiathiopthene (I)[1] and 2-methyl-4-phenyl-6a-thiathiophthene (II)[2] is given in Fig. 2. The bond lengths given for I include corrections for

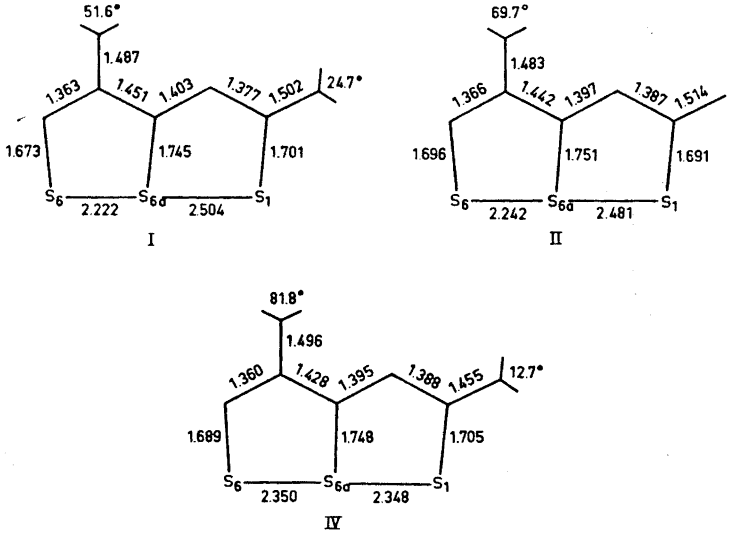


Fig. 2. Comparison of bond lengths in 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene (IV) with bond lengths in 2,4-diphenyl-6a-thiathiophene (I) and 2-methyl-4-phenyl-6a-thiathiophthene (II).

rigid-body libration, and they are therefore somewhat different from those given in Ref. 1. The standard deviations found for the bond lengths in I are ± 0.003, ± 0.005 to ± 0.007, and ± 0.007 to ± 0.011 Å, for S–S, S–C, and C–C, respectively, and the standard deviations for the bond lengths in II are ± 0.002 Å for S–S, ± 0.005 Å for S–C, and ± 0.006 to ± 0.008 Å for C–C.

There is close agreement between corresponding C–C bond lengths and also between corresponding C–S bond lengths in the 6a-thiathiophthene system of the three molecules (*cf.* Fig. 2). The S–S bond lengths, however, are equal in the present structure and unequal in the structures I and II. The lengths of S(1)–S(6a) and S(6a)–S(6) in compounds IV, I and II are 2.348 and 2.350 ± 0.0013 Å, 2.504 and 2.222 ± 0.003 Å, and 2.481 and 2.242 ± 0.002 Å, respectively. Thus the introduction of a *p*-dimethylamino group in the 2-phenyl group in compound I causes a pronounced change in the sulphur-sulphur bonding.

The ultraviolet spectra of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene and 2,4-diphenyl-6a-thiathiopthene in hexane are shown in Fig. 3. One notes that the introduction of the *p*-dimethylamino group leads to bathochromic shifts of the absorption maxima. Such red shifts are often observed when, as in the present case, the substituent atom has a lone pair of electrons which participates in the π-bonding system of the molecule.[10] Thus, in compound IV, π-electrons can be transferred from the nitrogen atom towards the 6a-thiathiophthene system of the molecule.

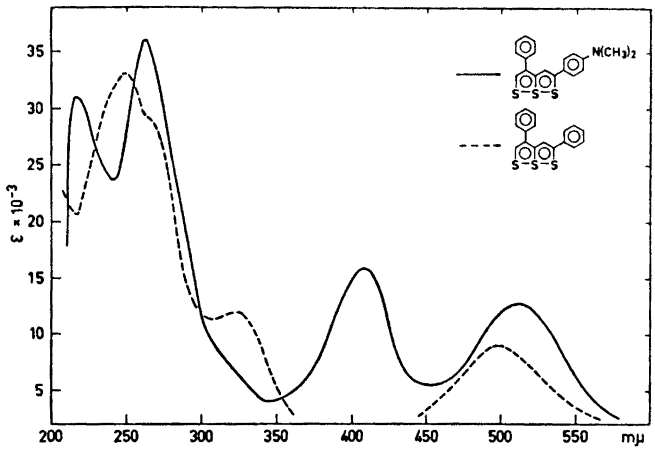


Fig. 3. Ultraviolet spectra of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene and 2,4-diphenyl-6a-thiathiophthene in hexane.

The results from CNDO/2 calculations on 6a-thiathiophthene and on monophenyl and monomethyl substituted 6a-thiathiophthenes,[11–13] show for the bonding in the three sulphur sequence that the σ-electron density on a terminal sulphur atom decreases when the π-electron density on this atom increases. Furthermore from these calculations there is a correlation between the σ-electron density on the terminal sulphur atoms and the lengths of the S–S bonds; the terminal sulphur atom with the lowest σ-electron density forms a shorter bond with the central sulphur atom than does the other terminal sulphur atom.

It seems likely from the above that the presence of the *p*-dimethylanilino group causes an increase in the π-electron density on S(1) in compound IV relative to the π-electron density on S(1) in compound I. As a result, the σ-electron density on S(1) in IV decreases and the S(1)–S(6a) bond becomes shorter than the corresponding bond in compound I.

The arrangement of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene molecules in the unit cell as seen along the *b*-axis and along the *a*-axis is shown in Figs. 4a and 4b. There are no intermolecular atomic distances shorter than corresponding van der Waals distances.

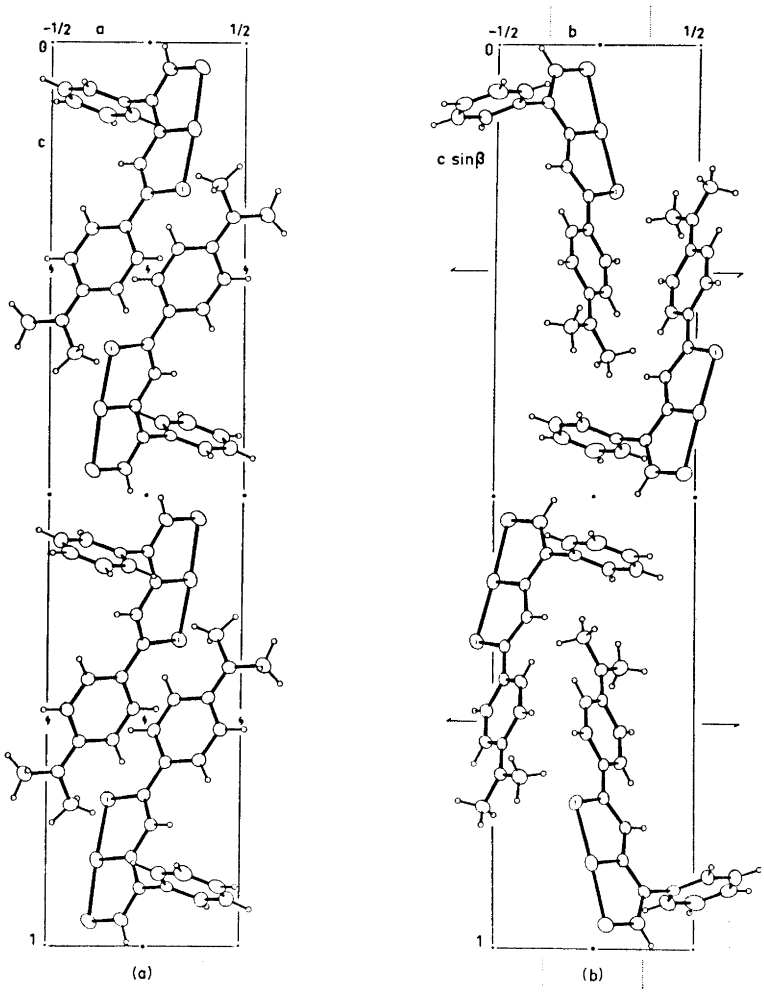


Fig. 4. The arrangement of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophene molecules as seen along the *b*-axis (a), and along the *a*-axis (b).

EXPERIMENTAL

The unit cell dimensions for crystals of 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene were determined from the 2θ values for 15 high order reflections. The 2θ values were measured at room temperature, $t = 22°C$, on the diffractometer using Cu$K\alpha$ radiation. A least squares procedure gave $a = 7.158(1)$ Å, $b = 7.413(1)$ Å, $c = 33.237(3)$ Å, and $\beta = 90.14(5)°$.

The molecular weight of the compound ($C_{19}H_{17}S_3N$) is 355.54, and four molecules per unit cell give a calculated density of 1.338 g/cm³, as compared with the density, 1.332 g/cm³, found by flotation.

The intensities of the reflections were collected on the diffractometer by means of the five-value scan technique.[14] Reflections for which the net count was greater than two times the respective standard deviations in the net count were accepted as observed. Unobserved reflections were neglected in order to save computing time.

Lp corrections and absorption corrections were applied, the latter according to a procedure of Coppens, Leiserowitz and Rabinovich.[15] The dimensions of the crystal were $0.26 \times 0.26 \times 0.05$ mm in the three axial directions; $\mu_{CuK\alpha} = 36.6$ cm^{-1}. A grid of $12 \times 12 \times 4$ points was used.

The scattering factors used for sulphur, nitrogen, and carbon were those given in the *International Tables*.[16] For hydrogen, the scattering factor curve given by Stewart *et al.*[17] was used.

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

Atom	x	y	z
S(1)	−0.18199(12)	0.58992(11)	0.33871(3)
S(6a)	−0.23843(11)	0.50912(10)	0.40575(3)
S(6)	−0.27678(12)	0.43648(12)	0.47390(3)
C(2)	0.00519(37)	0.45032(31)	0.33370(8)
C(3)	0.04220(37)	0.34084(34)	0.36648(8)
C(3a)	−0.05753(34)	0.35223(32)	0.40232(8)
C(4)	−0.01558(35)	0.24582(35)	0.43685(8)
C(5)	−0.10834(43)	0.27811(44)	0.47173(10)
C(6)	0.11526(35)	0.45136(31)	0.29704(8)
C(7)	0.05417(41)	0.53849(36)	0.26202(9)
C(8)	0.15899(40)	0.54198(36)	0.22759(9)
C(9)	0.33456(38)	0.45850(31)	0.22547(8)
C(10)	0.39702(44)	0.37091(37)	0.26061(9)
C(11)	0.28977(41)	0.36765(36)	0.29461(9)
C(12)	0.61649(57)	0.37084(60)	0.18926(14)
C(13)	0.37256(61)	0.55396(50)	0.15566(11)
C(14)	0.12777(37)	0.10048(36)	0.43512(7)
C(15)	0.30630(46)	0.13107(51)	0.44911(10)
C(16)	0.43638(55)	−0.00594(69)	0.44866(12)
C(17)	0.38842(62)	−0.17331(61)	0.43481(11)
C(18)	0.21298(64)	−0.20449(51)	0.42023(11)
C(19)	0.08357(48)	−0.06711(40)	0.42039(10)
N	0.44092(32)	0.46619(28)	0.19172(7)
H(3)	0.1415(34)	0.2483(34)	0.3663(7)
H(5)	−0.0792(39)	0.2085(39)	0.4965(9)
H(7)	−0.0654(41)	0.5970(35)	0.2619(9)
H(8)	0.1095(41)	0.5995(37)	0.2032(9)
H(10)	0.5194(38)	0.3135(37)	0.2603(8)
H(11)	0.3362(37)	0.3147(36)	0.3168(8)
H(121)	0.7022(62)	0.4123(55)	0.2095(14)
H(122)	0.6680(64)	0.3820(56)	0.1624(15)
H(123)	0.5967(50)	0.2500(56)	0.1926(11)
H(131)	0.3400(41)	0.6786(41)	0.1623(9)
H(132)	0.4707(54)	0.5624(44)	0.1354(12)
H(133)	0.2608(53)	0.5000(47)	0.1464(12)
H(15)	0.3357(42)	0.2405(43)	0.4573(9)
H(16)	0.5519(55)	0.0215(48)	0.4598(12)
H(17)	0.4787(53)	−0.2722(59)	0.4348(11)
H(18)	0.1791(54)	−0.3233(59)	0.4115(12)
H(19)	−0.0471(48)	−0.0862(41)	0.4092(10)

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

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
S(1)	814(6)	660(5)	786(6)	352(4)	146(4)	100(4)
S(6a)	621(4)	563(5)	918(6)	225(3)	−85(4)	98(4)
S(6)	794(6)	879(6)	762(6)	285(4)	−76(4)	267(4)
C(2)	600(16)	413(15)	600(16)	76(12)	− 4(12)	−59(13)
C(3)	568(16)	446(15)	565(16)	105(12)	−29(12)	12(13)
C(3a)	505(15)	430(15)	588(16)	81(11)	−59(12)	22(13)
C(4)	538(16)	532(16)	536(16)	48(12)	−85(12)	76(13)
C(5)	734(21)	791(22)	632(20)	177(16)	−18(16)	162(17)
C(6)	567(16)	389(15)	575(16)	33(11)	25(12)	−15(13)
C(7)	578(17)	537(18)	654(18)	64(13)	42(14)	−76(15)
C(8)	625(18)	547(18)	585(17)	24(13)	81(14)	−70(15)
C(9)	605(16)	386(16)	570(16)	−30(11)	−21(12)	−39(13)
C(10)	640(18)	582(19)	632(19)	131(14)	88(14)	37(15)
C(11)	662(19)	553(18)	593(18)	147(13)	138(14)	−20(15)
C(12)	787(25)	801(29)	808(27)	148(19)	88(21)	136(22)
C(13)	849(25)	729(25)	592(20)	−30(19)	87(17)	−29(19)
C(14)	563(16)	606(17)	402(13)	124(12)	−8(12)	57(12)
C(15)	638(20)	891(26)	782(23)	159(18)	−234(20)	−38(17)
C(16)	705(25)	1399(38)	789(25)	378(25)	−142(25)	−69(20)
C(17)	1028(31)	1017(30)	657(22)	561(25)	135(20)	202(21)
C(18)	1149(33)	601(23)	879(26)	245(21)	−45(19)	130(23)
C(19)	794(22)	576(19)	726(21)	137(16)	−86(15)	−21(17)
N	669(15)	570(15)	558(14)	11(11)	52(11)	10(12)

Atom	U	Atom	U	Atom	U
H(3)	874(96)	H(15)	750(104)	H(122)	1504(172)
H(5)	590(71)	H(16)	1250(189)	H(123)	1110(141)
H(7)	763(90)	H(17)	1381(135)	H(131)	828(101)
H(8)	892(94)	H(18)	1446(155)	H(132)	1111(127)
H(10)	793(91)	H(19)	1072(110)	H(133)	1111(128)
H(11)	663(85)	H(121)	1576(181)		

Table 5. Results from the rigid-body analysis of the 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene molecule.

	Eigenvalues	Eigenvectors Direction cosines × 10^4 relative to a, b, and c^*, respectively.		
Librational tensor, **L**	20.7(°)^2	−3010	−2831	9106
	3.2	−9213	3326	−2012
	2.2	−2458	−8997	−3608
Translational tensor, **T**	0.0643 Å^2	−4446	−3933	8048
	0.0501	8600	636	5062
	0.0369	2504	9173	3099
Symmetrized screw tensor, **S**		$\begin{pmatrix} -201 & -115 & -40 \\ & 87 & -46 \\ & & 114 \end{pmatrix}$ × 10^5 rad. Å		

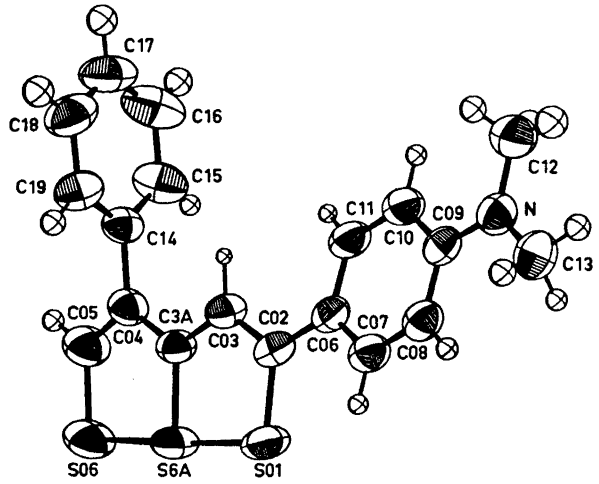


Fig. 5. The thermal ellipsoid plot showing the anisotropic vibration of the non-hydrogen atoms and the isotropic vibration of the hydrogen atoms. The latter has been scaled down by a factor of 4.

Table 6. Librational tensors from the rigid body analysis of certain parts of the 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene molecule. $\mathbf{L}_T$ refer to the 6a-thiathiophthene system plus C(6) and C(14), $\mathbf{L}_A$ refer to the *p*-dimethylanilino group plus C(2), and $\mathbf{L}_P$ refer to the phenyl group plus C(4).

	Eigenvalues	Eigenvectors Direction cosines × 10^4 relative to *a*, *b*, and *c*,* respectively.		
$\mathbf{L}_T$	17.5 (°)²	−6347	2359	7359
	4.9	−6462	3601	−6729
	3.1	−4237	−9026	−761
$\mathbf{L}_A$	55.0	5371	552	−8416
	5.4	1371	9788	1521
	4.1	8322	−1968	5183
$\mathbf{L}_P$	97.8	7328	−6535	−1896
	25.3	1974	4709	−8598
	9.4	6512	5926	4741

The full-matrix least squares program which was applied minimizes the function

$$D = \sum w[|F_o| - (1/K)|F_c|]^2$$

The weights were taken to be

$$w = 1/\sigma^2 (F_o)$$

where

$$\sigma^2(F_o) = F_o^2[I_{total} + I_{background} + (kI_{net})^2]/4I_{net}^2$$

In the latter expression k is the relative standard deviation in the scaling curve from the reference reflections. It was estimated to be 0.015 and 0.011 for the reference reflections 5,0,2 and 0,2,11, respectively, and the highest value was used.

Table 7. Observed and calculated structure factors for 2-(*p*-dimethylanilino)-4-phenyl-6a-thiathiophthene. The values given are ten times the absolute values. Unobserved reflections are not included.

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)
0	0	2	31	-31	6	0	6	214	213	-5	1	30	38	40	-1	1	5	732	752	2	1	3	373	-358
0	0	4	95	93	6	0	8	50	50	-5	1	31	41	-43	-1	1	6	356	353	2	1	4	469	476
0	0	6	503	-515	6	0	12	69	66	-5	1	33	70	-71	-1	1	7	570	580	2	1	5	453	466
0	0	8	1101	-1128	6	0	14	127	122	-4	1	0	141	-141	-1	1	8	26	-24	2	1	6	786	-792
0	0	10	394	-369	6	0	16	45	21	-4	1	1	311	306	-1	1	9	392	-396	2	1	7	129	129
0	0	12	476	464	6	0	18	369	355	-4	1	2	57	51	-1	1	10	282	-290	2	1	8	152	151
0	0	14	560	-562	6	0	20	227	-213	-4	1	5	123	128	-1	1	11	95	-86	2	1	9	231	231
0	0	16	179	-185	6	0	22	59	-65	-4	1	6	55	-52	-1	1	12	53	-46	2	1	10	52	-52
0	0	20	27	11	6	0	24	30	-30	-4	1	7	43	-47	-1	1	13	598	616	2	1	11	37	-50
0	0	22	245	-242	7	0	0	61	63	-4	1	9	45	52	-1	1	14	261	-266	2	1	12	243	-243
0	0	24	161	-165	7	0	2	41	34	-4	1	10	54	-51	-1	1	16	228	214	2	1	15	117	-84
0	0	26	84	-74	7	0	4	251	240	-4	1	11	426	423	-1	1	17	116	-112	2	1	16	104	-104
0	0	28	316	-320	7	0	6	68	-70	-4	1	12	198	-195	-1	1	18	383	395	2	1	17	566	556
0	0	30	283	268	7	0	16	63	61	-4	1	13	156	152	-1	1	19	96	104	2	1	18	66	-62
0	0	32	157	152	7	0	20	79	-68	-4	1	14	63	59	-1	1	20	275	276	2	1	19	69	-64
0	0	34	41	36	7	0	22	55	-59	-4	1	15	252	-296	-1	1	21	168	167	2	1	20	34	35
0	0	36	56	53	7	0	24	26	37	-4	1	16	195	194	-1	1	22	62	63	2	1	21	37	-38
1	0	0	650	660	8	0	2	57	65	-4	1	19	137	-142	-1	1	23	115	-117	2	1	22	122	119
1	0	2	366	-356	8	0	4	38	-36	-4	1	20	81	77	-1	1	24	195	201	2	1	23	167	162
1	0	4	368	-369	8	0	6	61	-48	-4	1	21	137	-142	-1	1	25	121	123	2	1	24	45	40
1	0	6	56	53	8	0	8	54	-62	-4	1	22	121	128	-1	1	26	185	-189	2	1	25	87	81
1	0	8	352	-351	8	0	10	51	48	-4	1	24	50	72	-1	1	27	249	-242	2	1	27	31	17
1	0	10	503	-505	8	0	16	28	-19	-4	1	25	265	-267	-1	1	28	161	-165	2	1	29	78	77
1	0	12	114	-116	-8	1	1	26	13	-4	1	27	117	-119	-1	1	29	238	-233	2	1	30	54	-58
1	0	14	1026	-1057	-8	1	3	34	20	-4	1	30	72	-77	-1	1	30	33	-40	2	1	31	57	-39
1	0	16	40	-42	-8	1	6	35	35	-4	1	31	67	71	-1	1	31	46	-50	2	1	33	156	-159
1	0	18	434	420	-8	1	8	44	38	-4	1	32	31	-45	-1	1	32	43	45	2	1	34	72	69
1	0	20	165	-177	-8	1	9	89	87	-3	1	0	187	-183	-1	1	35	68	-63	2	1	38	29	34
1	0	24	148	145	-8	1	10	38	-38	-3	1	1	515	-502	-1	1	37	27	27	2	1	39	22	-21
1	0	26	62	46	-8	1	11	85	74	-3	1	2	342	340	-1	1	40	37	-41	3	1	0	180	183
1	0	30	509	501	-8	1	12	49	-27	-3	1	3	280	271	0	1	1	472	473	3	1	1	562	566
1	0	32	95	-80	-8	1	13	42	-43	-3	1	4	88	76	0	1	2	238	250	3	1	2	467	470
2	0	0	501	-521	-8	1	14	40	36	-3	1	5	33	35	0	1	3	271	-277	3	1	3	283	287
2	0	2	596	-607	-8	1	16	24	2	-3	1	6	27	-22	0	1	4	381	401	3	1	5	52	52
2	0	4	60	-54	-7	1	0	59	57	-3	1	7	130	-124	0	1	6	398	401	3	1	6	46	-37
2	0	6	314	-323	-7	1	1	61	-61	-3	1	8	430	422	0	1	7	798	816	3	1	7	145	-145
2	0	8	251	-242	-7	1	2	59	58	-3	1	9	24	-6	0	1	8	314	319	3	1	9	338	340
2	0	10	216	-205	-7	1	3	37	-39	-3	1	10	218	-205	0	1	9	516	516	3	1	10	66	-64
2	0	12	118	-115	-7	1	6	182	172	-3	1	11	370	-365	0	1	10	768	800	3	1	11	118	112
2	0	14	28	-2	-7	1	7	160	149	-3	1	12	59	-58	0	1	11	474	486	3	1	12	39	-35
2	0	16	1129	1122	-7	1	9	48	42	-3	1	13	637	-643	0	1	12	57	53	3	1	13	278	269
2	0	18	134	167	-7	1	11	100	-94	-3	1	14	140	146	0	1	14	163	-161	3	1	14	64	70
2	0	20	42	-22	-7	1	13	79	-75	-3	1	15	128	-137	0	1	15	900	-890	3	1	15	240	232
2	0	24	94	-95	-7	1	15	51	-49	-3	1	17	160	101	0	1	17	558	-546	3	1	16	93	-78
2	0	26	41	-37	-7	1	17	116	-112	-3	1	18	204	-207	0	1	21	164	-162	3	1	18	26	-23
2	0	28	111	108	-7	1	19	35	-36	-3	1	19	54	-64	0	1	22	63	61	3	1	19	418	-412
2	0	30	44	67	-7	1	21	41	-35	-3	1	21	30	26	0	1	23	56	-55	3	1	20	165	163
2	0	32	60	-49	-7	1	23	96	-90	-3	1	23	37	-32	0	1	24	44	51	3	1	23	39	-33
2	0	34	81	-52	-7	1	24	26	-14	-3	1	25	81	-81	0	1	25	73	89	3	1	25	72	-72
2	0	36	26	-15	-6	1	3	137	-135	-3	1	26	77	82	0	1	26	73	-72	3	1	26	85	83
3	0	0	240	234	-6	1	4	96	92	-3	1	27	36	11	0	1	27	421	-419	3	1	28	49	-50
3	0	2	575	606	-6	1	5	89	-87	-3	1	28	55	-60	0	1	28	243	-250	3	1	29	65	-49
3	0	4	606	617	-6	1	6	133	129	-3	1	29	262	273	0	1	29	233	223	3	1	30	27	-19
3	0	6	61	64	-6	1	7	65	60	-3	1	30	48	-55	0	1	31	54	48	3	1	31	40	-40
3	0	10	63	-58	-6	1	8	120	115	-3	1	31	29	39	0	1	32	53	-53	3	1	32	27	20
3	0	12	216	-202	-6	1	9	514	-499	-3	1	32	31	-34	0	1	33	81	80	3	1	35	35	27
3	0	14	205	200	-6	1	10	95	-92	-3	1	33	33	41	0	1	36	39	36	3	1	36	44	-43
3	0	16	97	88	-6	1	11	38	40	-3	1	35	51	55	0	1	37	41	35	4	1	0	135	141
3	0	18	67	60	-6	1	12	67	-59	-3	1	37	28	21	0	1	39	30	18	4	1	1	707	704
3	0	20	143	-136	-6	1	13	36	33	-3	1	38	21	22	1	1	0	101	106	4	1	2	173	167
3	0	22	75	67	-6	1	14	185	-180	-2	1	0	74	73	1	1	1	503	507	4	1	3	88	-88
3	0	24	68	-64	-6	1	15	139	143	-2	1	1	451	-505	1	1	2	1061	1081	4	1	4	40	-42
3	0	26	46	-35	-6	1	16	95	-90	-2	1	2	262	263	1	1	3	2540	-2686	4	1	5	308	-307
3	0	28	120	-109	-6	1	17	42	33	-2	1	3	19	11	1	1	4	407	402	4	1	6	115	121
3	0	30	21	-15	-6	1	19	36	12	-2	1	4	349	-353	1	1	5	213	222	4	1	7	135	-129
3	0	34	40	32	-6	1	20	75	-71	-2	1	5	340	-357	1	1	6	52	58	4	1	8	91	93
3	0	36	24	25	-6	1	21	38	-31	-2	1	6	63	65	1	1	7	324	-322	4	1	9	44	48
4	0	0	90	97	-6	1	23	37	33	-2	1	7	46	-53	1	1	8	45	-41	4	1	10	91	-88
4	0	2	638	676	-6	1	24	37	40	-2	1	8	2721	-2651	1	1	9	275	-287	4	1	11	119	-116
4	0	4	669	-675	-6	1	25	159	152	-2	1	9	37	-49	1	1	10	157	162	4	1	12	171	172
4	0	6	151	-164	-6	1	26	35	-31	-2	1	10	417	-415	1	1	11	93	84	4	1	13	82	80
4	0	8	124	115	-6	1	27	89	97	-2	1	11	919	-921	1	1	12	158	158	4	1	14	182	-176
4	0	12	50	-40	-5	1	0	120	-116	-2	1	12	158	-151	1	1	13	805	-823	4	1	15	191	-184
4	0	14	166	-161	-5	1	1	108	100	-2	1	13	514	493	1	1	14	402	-399	4	1	16	107	-106
4	0	16	191	-183	-5	1	2	234	-222	-2	1	14	278	274	1	1	15	301	-303	4	1	17	246	-242
4	0	18	145	-136	-5	1	3	59	64	-2	1	15	402	432	1	1	16	73	73	4	1	18	35	24
4	0	20	40	24	-5	1	4	49	-41	-2	1	16	42	36	1	1	17	176	182	4	1	20	61	59
4	0	22	66	67	-5	1	5	40	38	-2	1	17	339	340	1	1	18	122	-129	4	1	21	96	90
4	0	30	41	24	-5	1	6	101	-95	-2	1	18	102	100	1	1	19	276	271	4	1	22	94	-88
4	0	32	63	48	-5	1	7	116	-110	-2	1	19	61	53	1	1	20	171	-170	4	1	23	58	-51
5	0	0	92	87	-5	1	8	52	-50	-2	1	20	43	54	1	1	21	117	113	4	1	29	68	-68
5	0	2	323	-325	-5	1	9	162	-153	-2	1	21	143	151	1	1	22	51	51	4	1	31	133	121
5	0	4	587	-573	-5	1	10	36	25	-2	1	22	147	-143	1	1	23	33	25	4	1	32	64	61
5	0	8	108	111	-5	1	11	244	240	-2	1	25	52	34	1	1	26	121	-122	5	1	0	111	116
5	0	10	32	-20	-5	1	12	229	-222	-2	1	26	28	23	1	1	28	43	-54	5	1	1	39	-38
5	0	12	56	-72	-5	1	13	427	423	-2	1	27	170	173	1	1	29	117	103	5	1	2	84	-87
5	0	16	97	-99	-5	1	15	85	81	-2	1	28	61	-57	1	1	30	91	-91	5	1	3	355	-358
5	0	18	227	208	-5	1	19	52	44	-2	1	29	29	41	1	1	31	183	192	5	1	5	362	-372
5	0	20	85	80	-5	1	21	44	-43	-2	1	30	34	25	1	1	32	95	95	5	1	6	184	-187
5	0	22	65	-67	-5	1	22	82	87	-2	1	31	110	-110	1	1	33	95	-89	5	1	7	168	169
5	0	26	95	89	-5	1	23	157	160	-2	1	32	134	138	1	1	34	54	49	5	1	8	113	-113
5	0	28	45	25	-5	1	24	56	64	-2	1	37	34	-34	1	1	36	63	69	5	1	9	66	-68
5	0	30	50	46	-5	1	25	65	65	-1	1	0	105	-106	1	1	37	39	40	5	1	10	30	-30
5	0	32	48	50	-5	1	26	39	37	-1	1	1	714	712	1	1	39	25	-23	5	1	11	86	-84
6	0	0	115	-114	-5	1	27	102	-91	-1	1	2	112	-115	2	1	0	74	-73	5	1	13	79	78
6	0	2	259	-263	-5	1	28	60	51	-1	1	3	820	829	2	1	1	1082	-1121	5	1	15	288	-281
6	0	4	41	-41	-5	1	29	66	-70	-1	1	4	143	140	2	1	2	437	456	5	1	16	97	-90

Table 7. 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)
5	1	17	254	244	-5	2	17	146	152	-1	2	6	117	-115	2	2	14	35	41	6	2	6	166	166
5	1	18	125	122	-5	2	18	33	-21	-1	2	7	201	-201	2	2	16	501	503	6	2	7	106	-105
5	1	19	108	101	-5	2	23	185	191	-1	2	8	74	-73	2	2	17	41	-42	6	2	8	38	46
5	1	21	44	41	-5	2	24	65	64	-1	2	9	180	-179	2	2	18	73	76	6	2	9	108	111
5	1	23	33	-13	-5	2	26	34	-24	-1	2	10	49	43	2	2	19	48	-48	6	2	11	80	83
5	1	24	25	12	-5	2	27	51	44	-1	2	11	377	386	2	2	20	28	13	6	2	13	49	-48
5	1	30	26	28	-5	2	28	127	-124	-1	2	12	455	477	2	2	21	140	142	6	2	18	151	155
5	1	31	47	53	-5	2	29	108	102	-1	2	13	327	335	2	2	22	44	39	6	2	19	49	55
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6	1	0	38	39	-4	2	0	247	244	-1	2	16	80	-75	2	2	26	66	63	6	2	27	25	-18
6	1	1	148	-150	-4	2	1	264	-255	-1	2	17	81	-77	2	2	27	89	76	7	2	2	62	57
6	1	3	42	-39	-4	2	2	29	34	-1	2	18	25	-39	2	2	29	51	51	7	2	4	152	154
6	1	4	45	40	-4	2	3	105	97	-1	2	19	111	115	2	2	30	103	-91	7	2	7	35	-46
6	1	5	192	191	-4	2	4	42	47	-1	2	20	120	-122	2	2	32	138	-126	7	2	8	56	-56
6	1	6	42	-43	-4	2	5	119	-116	-1	2	21	90	-84	2	2	33	173	174	7	2	9	67	71
6	1	7	150	150	-4	2	6	59	55	-1	2	22	76	-79	2	2	35	79	-77	7	2	11	39	46
6	1	8	161	-167	-4	2	7	73	74	-1	2	24	161	170	2	2	37	40	-40	7	2	18	32	-28
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6	1	15	69	62	-4	2	12	92	90	-1	2	28	65	-47	3	2	2	446	460	8	2	1	39	46
6	1	16	50	55	-4	2	13	67	-70	-1	2	29	48	43	3	2	3	40	-43	8	2	2	49	54
6	1	17	81	70	-4	2	14	421	-424	-1	2	30	143	-142	3	2	4	622	631	8	2	4	38	-40
6	1	18	81	83	-4	2	15	528	526	-1	2	31	40	42	3	2	5	278	-284	8	2	5	42	-43
6	1	19	104	103	-4	2	16	263	-262	-1	2	32	39	-50	3	2	6	267	265	8	2	6	39	-34
6	1	20	58	55	-4	2	18	136	-140	-1	2	33	70	-66	3	2	7	59	65	8	2	7	37	33
6	1	21	95	-98	-4	2	21	59	60	-1	2	35	86	-93	3	2	8	90	90	8	2	10	26	20
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7	1	3	86	79	-4	2	33	21	-23	0	2	2	583	-598	3	2	14	264	266	-8	3	9	59	66
7	1	4	68	73	-3	2	0	175	-164	0	2	4	101	93	3	2	15	117	117	-8	3	10	67	-70
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7	1	24	24	-26	-3	2	10	90	-84	0	2	15	76	83	3	2	28	108	-106	-7	3	12	94	92
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8	1	2	37	39	-3	2	12	199	-203	0	2	17	511	509	3	2	30	75	-66	-7	3	14	105	101
8	1	3	27	25	-3	2	13	123	125	0	2	19	209	-205	3	2	31	62	57	-7	3	15	38	-40
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-8	2	10	129	127	-3	2	23	138	-135	0	2	28	212	-222	4	2	3	154	150	-6	3	3	41	39
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-8	2	12	44	43	-3	2	26	43	37	0	2	32	25	20	4	2	5	70	-69	-6	3	10	53	-51
-8	2	13	43	47	-3	2	27	57	-57	0	2	33	84	-84	4	2	6	35	27	-6	3	11	59	-50
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-7	2	7	153	153	-3	2	32	36	39	1	2	2	1278	-1353	4	2	12	158	161	-6	3	16	109	-114
-7	2	8	38	24	-3	2	33	63	63	1	2	3	1564	1631	4	2	13	158	155	-6	3	17	82	87
-7	2	11	56	57	-3	2	34	25	24	1	2	4	111	-107	4	2	14	127	-131	-6	3	20	128	-129
-7	2	12	120	-122	-3	2	37	56	50	1	2	5	508	-522	4	2	15	214	-217	-6	3	22	31	-31
-7	2	13	107	103	-2	2	0	542	-540	1	2	6	203	-212	4	2	16	200	-185	-6	3	25	56	59
-7	2	14	80	-87	-2	2	1	414	356	1	2	7	135	-137	4	2	17	27	-13	-6	3	26	34	-30
-7	2	21	55	-60	-2	2	2	644	-633	1	2	8	229	221	4	2	18	92	-84	-5	3	0	131	-129
-7	2	22	57	-55	-2	2	3	137	134	1	2	9	127	131	4	2	19	127	129	-5	3	1	228	226
-7	2	23	34	-32	-2	2	4	141	138	1	2	12	204	187	4	2	22	53	60	-5	3	2	254	-250
-6	2	1	162	-150	-2	2	5	263	-269	1	2	13	135	-135	4	2	23	116	-117	-5	3	3	142	134
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-6	2	10	175	-168	-2	2	13	88	88	1	2	22	38	-31	5	2	2	178	-185	-5	3	13	54	56
-6	2	12	58	-52	-2	2	14	137	146	1	2	23	32	-20	5	2	3	102	-107	-5	3	14	39	29
-6	2	13	35	-33	-2	2	15	268	-272	1	2	24	82	84	5	2	4	201	-196	-5	3	15	79	85
-6	2	14	67	69	-2	2	16	250	257	1	2	25	97	-95	5	2	5	194	204	-5	3	16	63	59
-6	2	15	74	-75	-2	2	17	343	-359	1	2	26	48	42	5	2	6	181	185	-5	3	17	123	-119
-6	2	16	34	35	-2	2	19	44	44	1	2	27	27	20	5	2	7	29	-10	-5	3	18	82	82
-6	2	19	84	-79	-2	2	20	67	73	1	2	28	38	24	5	2	8	56	58	-5	3	21	43	-55
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-6	2	24	62	60	-2	2	23	196	192	1	2	32	123	-121	5	2	12	178	-182	-5	3	24	37	40
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-6	2	26	101	108	-2	2	25	176	176	1	2	35	23	15	5	2	14	104	-99	-5	3	27	36	-36
-6	2	27	22	-27	-2	2	26	248	247	1	2	36	23	-17	5	2	15	336	-331	-5	3	28	98	96
-5	2	1	142	-137	-2	2	27	62	66	1	2	39	20	-15	5	2	16	245	-246	-5	3	29	73	-75
-5	2	2	44	53	-2	2	28	82	92	2	2	0	521	-540	5	2	17	35	41	-5	3	30	39	50
-5	2	3	47	55	-2	2	29	113	-124	2	2	1	226	232	5	2	18	173	168	-4	3	0	309	-303
-5	2	4	31	-24	-2	2	30	67	-62	2	2	2	173	-181	5	2	19	64	65	-4	3	1	239	240
-5	2	5	33	-40	-2	2	31	67	67	2	2	3	376	366	5	2	20	100	102	-4	3	3	70	-70
-5	2	6	82	79	-2	2	32	100	-110	2	2	4	99	104	5	2	23	32	23	-4	3	4	122	120
-5	2	7	161	-158	-2	2	34	64	-66	2	2	5	496	-519	5	2	25	45	39	-4	3	5	293	-277
-5	2	9	38	-36	-2	2	37	45	50	2	2	6	516	529	5	2	30	21	17	-4	3	6	76	-70
-5	2	11	215	-214	-1	2	0	132	-134	2	2	7	280	-282	5	2	31	21	23	-4	3	7	119	117
-5	2	12	435	435	-1	2	1	314	-313	2	2	8	194	-193	6	2	0	149	-150	-4	3	8	223	216
-5	2	13	148	-146	-1	2	2	431	440	2	2	9	65	-65	6	2	1	277	-296	-4	3	9	29	38
-5	2	14	36	-34	-1	2	3	553	-568	2	2	10	84	-96	6	2	2	240	-255	-4	3	10	165	163
-5	2	15	35	-41	-1	2	4	184	185	2	2	11	308	-310	6	2	3	82	-90	-4	3	11	140	134
-5	2	16	28	29	-1	2	5	207	-208	2	2	13	25	-24	6	2	4	40	35	-4	3	12	26	-19

Table 7. 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)
-4	3	14	276	270	-1	3	33	24	-22	3	3	8	391	397	8	3	4	26	-23	-3	4	28	49	48
-4	3	15	338	-342	-1	3	34	74	-75	3	3	9	440	-455	8	3	5	40	-39	-3	4	29	98	-94
-4	3	16	226	220	-1	3	35	45	50	3	3	10	93	-97	8	3	7	35	-43	-3	4	30	40	40
-4	3	18	74	67	-1	3	38	39	-40	3	3	11	154	152	8	3	8	35	39	-3	4	31	60	-63
-4	3	23	47	-46	0	3	1	281	285	3	3	12	343	352	-7	4	0	40	-36	-3	4	32	46	56
-4	3	24	38	-37	0	3	2	110	-113	3	3	13	271	270	-7	4	1	108	99	-2	4	0	52	-58
-4	3	25	54	-56	0	3	3	316	313	3	3	14	295	293	-7	4	2	112	-102	-2	4	1	399	381
-4	3	26	25	-36	0	3	4	252	263	3	3	15	69	60	-7	4	3	69	69	-2	4	2	299	-296
-4	3	27	48	-45	0	3	5	340	-347	3	3	16	99	-96	-7	4	4	39	-44	-2	4	3	123	-120
-4	3	28	62	65	0	3	6	255	255	3	3	18	75	-77	-7	4	5	27	-6	-2	4	4	596	572
-4	3	30	70	-62	0	3	7	227	-218	3	3	19	115	-112	-7	4	7	66	66	-2	4	5	100	-96
-4	3	31	31	46	0	3	9	196	-178	3	3	20	183	179	-7	4	9	28	-23	-2	4	6	285	276
-4	3	32	72	-78	0	3	10	366	361	3	3	21	59	61	-7	4	11	44	43	-2	4	7	137	-139
-4	3	35	46	52	0	3	11	444	437	3	3	26	145	150	-7	4	12	92	-94	-2	4	8	156	-156
-3	3	0	71	62	0	3	12	112	113	3	3	28	69	-67	-7	4	13	136	135	-2	4	9	282	-279
-3	3	1	365	-343	0	3	14	81	-84	3	3	29	160	-153	-7	4	14	128	-129	-2	4	10	182	-171
-3	3	2	409	410	0	3	15	80	-94	3	3	30	67	-68	-7	4	16	51	54	-2	4	11	219	-207
-3	3	3	125	-128	0	3	16	187	190	3	3	33	34	32	-6	4	0	122	-111	-2	4	12	119	-116
-3	3	4	142	146	0	3	17	62	-53	3	3	34	43	-39	-6	4	1	99	93	-2	4	14	27	23
-3	3	5	66	58	0	3	21	48	-39	3	3	35	52	55	-6	4	2	44	-42	-2	4	15	151	-155
-3	3	6	525	510	0	3	25	51	-38	4	3	0	283	303	-6	4	3	26	-23	-2	4	16	261	266
-3	3	9	44	43	0	3	26	65	-55	4	3	1	211	224	-6	4	4	88	86	-2	4	17	243	-252
-3	3	10	33	-29	0	3	27	89	-88	4	3	2	27	39	-6	4	5	30	15	-2	4	18	195	197
-3	3	11	261	-264	0	3	28	111	-116	4	3	3	54	57	-6	4	6	71	-72	-2	4	19	35	-10
-3	3	13	326	-323	0	3	29	58	53	4	3	4	58	-102	-6	4	8	28	23	-2	4	22	260	-273
-3	3	14	201	199	0	3	30	49	49	4	3	5	47	48	-6	4	9	82	-80	-2	4	23	63	-66
-3	3	15	193	-190	0	3	32	75	-73	4	3	6	167	168	-6	4	11	65	51	-2	4	24	91	90
-3	3	17	194	196	0	3	33	60	59	4	3	7	103	-103	-6	4	12	39	-36	-2	4	25	89	92
-3	3	18	355	-366	0	3	34	27	-33	4	3	8	173	176	-6	4	14	86	88	-2	4	26	54	-53
-3	3	19	171	178	0	3	36	44	37	4	3	9	88	98	-6	4	15	166	-165	-2	4	27	106	109
-3	3	20	67	-65	0	3	37	23	-21	4	3	10	52	53	-6	4	16	134	146	-2	4	28	49	-53
-3	3	21	66	-67	0	3	38	58	-60	4	3	11	32	46	-6	4	17	98	-101	-2	4	29	28	31
-3	3	24	205	-205	1	3	0	320	-329	4	3	12	401	408	-6	4	18	40	51	-2	4	30	29	-30
-3	3	25	72	-72	1	3	2	178	183	4	3	13	251	256	-6	4	19	29	30	-2	4	31	121	116
-3	3	24	215	-219	1	3	3	352	-359	4	3	14	30	-18	-6	4	20	69	-73	-2	4	32	46	-46
-3	3	25	84	82	1	3	4	40	-26	4	3	15	362	-361	-6	4	21	35	-34	-2	4	33	31	20
-3	3	27	99	99	1	3	5	355	350	4	3	16	131	-124	-5	4	0	67	66	-2	4	35	24	19
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-1	3	5	329	319	2	3	15	153	155	6	3	12	52	-51	-4	4	30	59	58	0	4	10	232	229
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-1	3	30	84	84	3	3	5	161	171	8	3	0	50	50	-3	4	23	58	-58	1	4	1	40	-44
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Table 7. 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)
1	4	4	73	75	4	4	24	40	-35	-4	5	13	36	38	0	5	32	43	-35	5	5	24	40	33
1	4	5	35	-27	4	4	25	57	-56	-4	5	14	75	83	0	5	33	49	44	6	5	0	74	-86
1	4	6	297	-264	4	4	26	77	-71	-4	5	15	108	-110	1	5	0	105	107	6	5	1	87	-98
1	4	8	373	361	4	4	27	73	-72	-4	5	16	34	-33	1	5	1	147	149	6	5	6	52	-50
1	4	9	32	-25	4	4	28	54	-51	-4	5	17	99	-105	1	5	2	112	120	6	5	9	30	27
1	4	10	85	-88	4	4	29	29	-31	-4	5	18	168	167	1	5	3	61	-63	6	5	10	63	-76
1	4	11	220	-215	4	4	30	37	32	-4	5	19	56	61	1	5	4	48	47	6	5	11	60	-66
1	4	12	82	-51	4	4	31	19	9	-4	5	21	143	150	1	5	5	169	-161	6	5	12	53	-63
1	4	13	168	-173	5	4	0	57	66	-4	5	23	26	9	1	5	6	245	234	6	5	13	43	-51
1	4	15	135	128	5	4	1	77	-76	-3	5	1	121	-115	1	5	7	179	186	6	5	14	59	69
1	4	16	63	61	5	4	2	55	-58	-3	5	2	149	150	1	5	8	110	107	6	5	15	63	68
1	4	18	254	-248	5	4	3	104	-104	-3	5	3	362	-353	1	5	9	280	276	6	5	16	67	66
1	4	20	83	80	5	4	4	33	-27	-3	5	4	194	187	1	5	10	150	-149	6	5	17	32	29
1	4	21	30	30	5	4	5	127	128	-3	5	7	283	274	1	5	11	171	-166	6	5	18	26	-34
1	4	22	117	-118	5	4	8	81	-87	-3	5	8	43	30	1	5	12	105	-116	6	5	19	44	-44
1	4	23	152	-151	5	4	10	105	110	-3	5	9	137	131	1	5	13	96	-101	7	5	1	47	57
1	4	24	113	-110	5	4	12	97	-102	-3	5	10	47	-43	1	5	14	63	-62	7	5	2	78	85
1	4	25	57	-55	5	4	13	75	-76	-3	5	12	66	-66	1	5	15	34	40	7	5	3	50	57
1	4	26	38	25	5	4	14	29	-23	-3	5	14	28	12	1	5	16	69	-71	7	5	5	30	-32
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1	4	28	72	70	5	4	16	54	-61	-3	5	18	96	-103	1	5	18	94	-95	-6	6	1	129	123
1	4	29	82	65	5	4	18	56	84	-3	5	19	160	167	1	5	19	53	49	-6	6	2	49	-50
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1	4	34	40	42	5	4	27	49	-48	-3	5	22	89	-86	1	5	23	105	-114	-6	6	5	93	-88
1	4	35	31	29	5	4	28	27	22	-3	5	24	108	-106	1	5	24	58	-58	-6	6	6	63	54
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2	4	8	248	-250	6	4	14	45	42	-2	5	7	150	148	2	5	7	149	143	-5	6	8	96	-94
2	4	9	375	-378	6	4	15	60	67	-2	5	8	29	-31	2	5	9	91	-96	-5	6	11	27	28
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3	4	19	180	182	-6	5	16	167	-171	-1	5	20	180	180	3	5	23	74	69	-3	6	13	28	-10
3	4	20	45	-48	-6	5	17	103	102	-1	5	21	54	-58	3	5	25	99	101	-3	6	14	37	34
3	4	21	38	41	-6	5	19	27	-23	-1	5	22	89	81	3	5	26	33	27	-3	6	15	39	34
3	4	22	91	-89	-5	5	1	76	69	-1	5	23	36	38	3	5	28	37	-31	-3	6	17	160	-171
3	4	23	43	-35	-5	5	2	67	-52	-1	5	25	36	47	3	5	29	64	-62	-3	6	18	87	90
3	4	24	86	90	-5	5	3	167	153	-1	5	27	44	-43	4	5	0	176	187	-3	6	19	88	91
3	4	25	27	-21	-5	5	4	105	-99	-1	5	29	38	46	4	5	1	33	27	-3	6	20	92	89
3	4	26	90	101	-5	5	7	28	-20	0	5	1	35	30	4	5	4	88	95	-3	6	21	169	-165
3	4	28	47	-40	-5	5	8	84	-84	0	5	2	96	-93	4	5	5	68	73	-3	6	22	34	-42
3	4	29	57	-58	-5	5	9	51	49	0	5	3	132	127	4	5	6	99	107	-3	6	23	44	52
3	4	30	24	19	-5	5	10	28	-37	0	5	4	60	55	4	5	7	110	-109	-3	6	24	30	-32
3	4	31	34	38	-5	5	12	30	-22	0	5	5	317	-311	4	5	9	82	83	-3	6	27	21	-8
3	4	32	32	31	-5	5	14	110	-100	0	5	6	173	175	4	5	11	91	97	-2	6	1	84	81
4	4	0	258	279	-5	5	15	66	66	0	5	7	175	-167	4	5	13	64	64	-2	6	2	40	-34
4	4	1	101	107	-5	5	17	144	-150	0	5	8	355	350	4	5	15	133	-128	-2	6	3	124	-120
4	4	4	72	-72	-5	5	18	110	119	0	5	9	155	164	4	5	22	74	-73	-2	6	4	218	218
4	4	5	125	137	-5	5	19	93	-92	0	5	10	40	51	4	5	23	93	93	-2	6	5	100	-102
4	4	6	117	-126	-5	5	20	123	127	0	5	11	143	133	4	5	24	35	38	-2	6	6	331	321
4	4	7	232	247	-5	5	21	23	14	0	5	12	57	51	4	5	26	52	-48	-2	6	7	222	-219
4	4	8	207	-217	-5	5	22	44	41	0	5	13	110	-107	4	5	27	50	-55	-2	6	9	27	17
4	4	9	135	147	-5	5	23	23	25	0	5	16	105	99	5	5	1	107	-130	-2	6	10	146	-143
4	4	11	162	-163	-5	5	24	24	29	0	5	17	52	-46	5	5	3	40	-52	-2	6	11	80	76
4	4	12	312	318	-4	5	0	202	-187	0	5	19	66	-61	5	5	4	68	87	-2	6	12	42	-47
4	4	13	207	205	-4	5	1	120	107	0	5	20	134	132	5	5	7	29	21	-2	6	14	62	-58
4	4	15	168	-172	-4	5	2	126	-112	0	5	21	144	144	5	5	9	140	149	-2	6	16	45	48
4	4	16	50	-36	-4	5	3	142	-146	0	5	22	64	-63	5	5	10	55	-62	-2	6	17	42	-36
4	4	17	33	31	-4	5	4	184	188	0	5	23	74	83	5	5	11	29	46	-2	6	19	58	-59
4	4	18	66	72	-4	5	5	322	-307	0	5	24	99	-112	5	5	12	140	-155	-2	6	20	68	-69
4	4	19	92	86	-4	5	7	58	61	0	5	25	103	-97	5	5	13	129	-139	-2	6	21	75	78
4	4	20	44	-48	-4	5	8	127	128	0	5	26	102	-104	5	5	15	27	-30	-2	6	22	44	-46
4	4	21	37	-30	-4	5	9	44	46	0	5	29	45	43	5	5	16	27	24	-2	6	27	24	15
4	4	22	48	48	-4	5	10	68	59	0	5	30	76	-61	5	5	18	26	-10	-2	6	28	30	-33

Table 7. 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)
-1	6	0	115	-112	1	6	24	87	-88	4	6	24	43	42	-2	7	5	128	126	1	7	10	111	-108
-1	6	1	67	64	1	6	25	28	34	5	6	1	52	-45	-2	7	6	98	-93	1	7	12	70	65
-1	6	4	135	137	1	6	30	27	-24	5	6	3	31	30	-2	7	7	74	70	1	7	14	53	43
-1	6	5	289	-278	2	6	1	27	-20	5	6	4	32	34	-2	7	8	56	-51	1	7	15	79	79
-1	6	6	78	-74	2	6	2	57	-58	5	6	6	28	-25	-2	7	9	64	-64	1	7	16	33	-27
-1	6	7	48	42	2	6	4	104	-103	5	6	8	73	77	-2	7	10	46	40	1	7	17	43	35
-1	6	8	154	-148	2	6	5	195	-196	5	6	10	90	101	-2	7	12	34	-22	1	7	19	45	39
-1	6	9	36	-34	2	6	6	172	169	5	6	11	51	-59	-2	7	13	29	3	1	7	20	29	-9
-1	6	13	62	71	2	6	7	264	264	5	6	12	111	-114	-2	7	17	32	29	1	7	21	41	42
-1	6	14	90	-88	2	6	8	165	162	5	6	13	64	-61	-2	7	18	90	-88	1	7	22	85	-80
-1	6	15	93	90	2	6	9	268	-270	5	6	14	94	-100	-2	7	19	59	-62	1	7	23	98	-100
-1	6	17	42	41	2	6	10	134	-135	5	6	15	37	45	-2	7	20	38	42	1	7	25	59	-63
-1	6	18	125	-125	2	6	11	42	-39	5	6	16	64	64	-2	7	21	30	-34	2	7	0	62	68
-1	6	19	95	91	2	6	12	66	-63	5	6	19	38	-42	-2	7	22	36	-31	2	7	3	83	82
-1	6	20	109	-105	2	6	13	38	34	6	6	0	103	-127	-2	7	23	28	-26	2	7	4	35	33
-1	6	21	91	88	2	6	15	48	-46	6	6	1	27	-16	-2	7	24	94	98	2	7	6	44	-34
-1	6	22	133	140	2	6	16	39	-43	6	6	2	24	26	-1	7	0	63	-66	2	7	7	178	178
-1	6	23	59	-66	2	6	17	37	-41	6	6	7	32	-34	-1	7	1	56	51	2	7	8	52	-43
-1	6	24	93	102	2	6	18	29	-22	6	6	8	58	58	-1	7	2	58	44	2	7	9	70	-73
-1	6	26	30	-29	2	6	19	42	43	6	6	9	26	27	-1	7	3	90	86	2	7	10	64	-60
0	6	0	60	-60	2	6	20	26	-27	6	6	10	44	-55	-1	7	4	142	-141	2	7	11	141	-145
0	6	1	104	106	2	6	22	76	-78	6	6	11	117	-133	-1	7	5	92	-89	2	7	12	84	87
0	6	4	119	-115	2	6	23	61	59	6	6	12	113	-128	-1	7	7	188	-190	2	7	19	25	26
0	6	5	38	39	2	6	26	66	66	-5	7	0	49	44	-1	7	8	44	40	2	7	20	40	-48
0	6	6	280	-280	2	6	27	22	14	-5	7	1	29	16	-1	7	9	109	-106	2	7	21	71	-69
0	6	7	269	264	2	6	29	22	-19	-5	7	2	28	-24	-1	7	10	150	153	2	7	23	37	-37
0	6	8	97	95	3	6	0	58	66	-5	7	3	160	158	-1	7	11	37	37	2	7	24	29	19
0	6	10	221	225	3	6	1	33	-39	-5	7	4	149	-150	-1	7	12	37	-36	3	7	2	27	-18
0	6	12	58	-49	3	6	2	39	-48	-5	7	5	32	27	-1	7	17	71	-65	3	7	3	31	-12
0	6	14	37	-32	3	6	3	58	-65	-5	7	6	33	35	-1	7	18	44	-41	3	7	4	35	37
0	6	15	75	75	3	6	5	43	38	-5	7	7	87	-91	-1	7	19	100	-99	3	7	5	43	44
0	6	16	28	27	3	6	7	50	-48	-5	7	8	41	41	-1	7	21	40	42	3	7	6	154	-162
0	6	17	48	37	3	6	8	94	-88	-5	7	11	31	-39	-1	7	22	30	25	3	7	7	115	-117
0	6	18	85	-81	3	6	10	76	-72	-4	7	1	51	55	-1	7	23	128	132	3	7	8	46	43
0	6	19	49	48	3	6	12	73	65	-4	7	2	66	-66	-1	7	24	21	-18	3	7	9	35	-36
0	6	20	118	123	3	6	13	53	54	-4	7	4	58	57	0	7	1	55	48	3	7	10	84	-83
0	6	21	31	-33	3	6	15	44	-53	-4	7	5	142	-136	0	7	3	55	-42	3	7	11	31	-23
0	6	22	213	215	3	6	16	48	-46	-4	7	6	84	81	0	7	4	155	-156	3	7	12	161	166
0	6	23	109	-107	3	6	18	33	27	-4	7	7	99	-94	0	7	5	249	-250	3	7	14	49	-50
0	6	25	45	-42	3	6	19	43	31	-4	7	9	57	57	0	7	6	80	-81	3	7	18	59	52
0	6	26	73	-75	3	6	20	47	-44	-4	7	9	42	40	0	7	7	157	-155	3	7	20	34	-38
1	6	0	104	-112	3	6	21	25	-23	-4	7	10	41	-41	0	7	8	179	178	3	7	21	58	-55
1	6	3	38	34	3	6	23	45	50	-4	7	14	41	49	0	7	9	154	159	4	7	4	45	44
1	6	4	178	-179	3	6	24	97	96	-4	7	17	116	-121	0	7	11	72	71	4	7	6	43	-43
1	6	5	111	111	3	6	25	29	26	-4	7	18	100	105	0	7	13	92	88	4	7	7	64	-64
1	6	6	98	100	4	6	0	88	101	-3	7	3	151	-148	0	7	14	48	52	4	7	9	90	89
1	6	7	217	210	4	6	2	35	-55	-3	7	4	84	85	0	7	17	46	-46	4	7	10	114	118
1	6	8	482	476	4	6	3	27	-26	-3	7	5	43	-28	0	7	18	82	-82	4	7	11	113	114
1	6	9	35	35	4	6	6	48	-54	-3	7	7	151	146	0	7	20	44	48	4	7	13	84	-89
1	6	10	126	123	4	6	9	156	171	-3	7	8	59	-58	0	7	21	118	121	4	7	14	56	-56
1	6	11	156	-155	4	6	10	183	193	-3	7	9	41	42	0	7	22	76	-71	4	7	15	31	33
1	6	12	143	-139	4	6	11	42	-42	-3	7	14	37	-29	0	7	23	50	47	4	7	16	27	27
1	6	13	44	-39	4	6	12	55	62	-3	7	16	48	46	0	7	26	38	44	4	7	17	23	16
1	6	16	69	-75	4	6	13	84	92	-3	7	18	59	-63	1	7	0	62	66	5	7	0	37	-44
1	6	17	30	-26	4	6	14	62	-61	-3	7	19	95	96	1	7	1	72	78	5	7	5	32	-27
1	6	19	73	-64	4	6	15	64	-67	-3	7	20	74	-70	1	7	2	88	90	5	7	6	46	-41
1	6	20	124	121	4	6	19	29	-26	-3	7	21	55	53	1	7	4	143	-139	5	7	7	35	46
1	6	21	29	33	4	6	21	62	-57	-3	7	22	27	-29	1	7	5	107	-107	5	7	8	95	106
1	6	22	26	32	4	6	22	37	42	-2	7	0	72	-68	1	7	6	58	59	5	7	9	105	118
1	6	23	165	-169	4	6	23	34	35	-2	7	2	96	94	1	7	7	112	109	5	7	10	34	41
										-2	7	3	37	-33	1	7	9	130	130	5	7	11	31	-28

Final atomic coordinates from the least squares refinement are listed in Table 3, and the temperature parameters are listed in Table 4. A pictorial representation of the thermal motion of the atoms is given in Fig. 5.[18] The final list of structure factors is given in Table 7.

An analysis of the thermal parameters of the S, N, and C atoms, assuming the whole molecule to be a rigid body, was carried out according to the method by Schomaker and Trueblood.[6] The rigid-body tensors arrived at are given in Table 5. The r.m.s. difference between observed and calculated U_{ij}'s is 0.0075 Å^2. Bond lengths which have been corrected according to the libration tensor **L** in Table 5 are given in the second column of Table 1.

Separate rigid body analyses for certain parts of the 2-(*p*-dimethylanilino)-4-phenyl 6a-thiathiophthene molecule have also been carried out. The parts of the molecule treated in this way are the 6a-thiathiophthene system plus C(6) and C(14), the *p*-dimethylanilino group plus C(2), and the phenyl group plus C(4). The corresponding librational tensors, $\mathbf{L}_T$, $\mathbf{L}_A$, and $\mathbf{L}_P$ from these calculations are listed in Table 6.

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 6a-thiathiophthene system plus C(6) and C(14), the r.m.s. difference of U_{ij}'s is 0.0037 Å^2. Similarly for the *p*-dimethylanilino group plus C(2), and for the phenyl group plus C(4), the r.m.s. differences are 0.0021 and 0.0028 Å^2, respectively.

Bond lengths which have been corrected according to the libration tensors $\mathbf{L}_T$, $\mathbf{L}_A$, and $\mathbf{L}_P$, respectively, are listed in the first column of Table 1.

The average C – C bond length in the phenyl group of the present structure is 1.373 Å from the *l* values in Table 1, 1.378 Å from the *l'* values, and 1.390 Å from the *l''* values. The C(2) – C(6) bond length became 1.455 Å when corrected according to $\mathbf{L}_T$ and the same value was obtained when the corrections were carried out according to $\mathbf{L}_A$. Corrections according to $\mathbf{L}_T$ and $\mathbf{L}_P$ resulted in slightly different values, 1.493 and 1.498 Å, for the C(4) – C(14) bond length. The average value, 1.496 Å, is given in the first column of Table 1.

The eigenvector of $\mathbf{L}_A$ corresponding to the largest libration, 7.4°, is directed roughly along C(2) – C(6) – N, and the eigenvector of $\mathbf{L}_P$ with largest libration amplitude, 9.9°, is directed along C(4) – C(14) – C(17).

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