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The Crystal and Molecular Structure of 2,5-Diphenyl-3,4-diaza-6a-thiathiophthene

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2,5-Diphenyl-3,4-diaza-6a-thiathiophthene crystallizes in the orthorhombic space group $Pc2_1n$, with unit cell dimensions: $a = 12.494(12)$ Å, $b = 4.007(8)$ Å, and $c = 28.185(15)$ Å. There are four molecules per unit cell.

The structure was solved by the heavy atom method, and refined by full matrix least squares. The refinement comprises 1039 $h0l - h3l$ reflections.

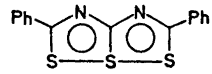
The 2- and 5-phenyl groups are twisted 2.0 and 7.0° about the respective connecting bonds, and the lengths of the S(1)–S(6a) and S(6a)–S(6) bonds are 2.319(3) and 2.328(3) Å, respectively, with the angle S(1)–S(6a)–S(6) = 174.3(2)°. The other bond lengths in the central ring system are S(1)–C(2) = 1.692(9) Å, S(6a)–C(3a) = 1.786(8) Å, S(6)–C(5) = 1.698(8) Å, C(2)–N(3) = 1.325(10) Å, N(3)–C(3a) = 1.330(9) Å, C(3a)–N(4) = 1.344(10) Å, and N(4)–C(5) = 1.336(10).

The C–C bonds connecting the phenyl groups to the 3,4-diaza-6a-thiathiophthene system are C(2)–C(12) = 1.515(11) Å and C(5)–C(6) = 1.475(11) Å.

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

There are no intermolecular close contacts between sulphur and neighbouring atoms or groups.

The present structure study of 2,5-diphenyl-3,4-diaza-6a-thiathiophthene (I) has been carried out in order to obtain further experimental evidence for the effect of phenyl substituents on the sulphur-sulphur bonding in 6a-thiathiophthenes.



(I)

STRUCTURE DETERMINATION

A brief account of the structure determination has been reported earlier,[1] and a more detailed description is given here.

Compound I was first described by Derocque, Perrier and Vialle.[2] The crystals are orange-red and belong to the orthorhombic space group $Pc2_1n$.

The structure analysis is based on photographic data, taken with Weissenberg camera and Cu$K\alpha$ radiation. 1039 $h0l-h3l$ reflections were observed.

The structure was solved by the heavy atom method and refined by a least squares procedure (see for example Ref. 7). The constants a_1 and a_2 in the weighting scheme were in the present case set equal to 1.0. Unobserved reflections with $K|F_c|$ greater than $F_o^{\text{threshold}}$ were included in the refinement with $F_o = F_o^{\text{threshold}}$. Anisotropic temperature factors were applied to sulphur, nitrogen, and carbon, and isotropic ones to hydrogen. Fourteen low order reflections whose intensities were very difficult to estimate, were excluded from the least squares refinement. The final R factor is 0.068 when unobserved reflections are included, and 0.065 when they are omitted.

A rigid-body analysis of the 2,5-diphenyl-3,4-diaza-6a-thiathiophthene molecule has been carried out according to the method of Schomaker and Trueblood,[3] and the S–S, S–C, N–C, and C–C bond lengths have been corrected for rigid-body libration according to Cruickshank's formula.[4] For further details with respect to the structure determination, see Experimental.

DISCUSSION

Molecular shape and dimensions. Bond lengths and angles in the 2,5-diphenyl-3,4-diaza-6a-thiathiophthene molecule are listed in Tables 1 and 2, and shown in Figs. 1a and 1b. Furthermore, in Fig. 1a the deviations for sulphur, nitrogen, and carbon from the least squares plane of the molecule are given. The equation for this plane, with neglect of hydrogen and triple weight on sulphur, is

$$0.20734X + 0.90184Y - 0.37908Z = -0.65397$$

where X, Y, and Z are in Å units. One notes with respect to the linear sequences C(2)–C(12)–C(15) and C(5)–C(6)–C(9), *cf.* Fig. 1a, that the former lies almost in the plane of the molecule and that the latter points slightly out of it.

The equation for the least squares plane through the atoms of the central ring system with triple weight on sulphur, is

$$0.21283X + 0.90443Y - 0.36974Z = -0.51717$$

and the deviations in Å units from this plane are S(1) 0.006, S(6a) −0.006, S(6) −0.003, C(2) −0.002, N(3) −0.015, C(3a) 0.008, N(4) −0.007, and C(5) 0.023. Thus, the 3,4-diaza-6a-thiathiophthene system is planar within the error.

The twist angle of the 2-phenyl group about C(2)–C(12) is 2.0°. The twist angle was taken as the angle between the plane through S(1), C(2), N(3), and C(12), and the plane through C(2), C(12), C(13), and C(17).

Table 1. Bond lengths (l) and standard deviations in bond lengths $\sigma(l)$ in 2,5-diphenyl-3,4-diaza-6a-thiathiophthene. Bond lengths (l') have been corrected for rigid-body libration.

Bond	l' (Å)	l (Å)	$\sigma(l)$ (Å)
S(1) – S(6a)	2.319	2.316	0.003
S(6a) – S(6)	2.328	2.325	0.003
S(1) – C(2)	1.692	1.691	0.009
S(6a) – C(3)	1.786	1.784	0.008
S(6) – C(5)	1.698	1.697	0.008
C(2) – N(3)	1.325	1.323	0.010
N(3) – C(3a)	1.330	1.328	0.009
C(3a) – N(4)	1.344	1.344	0.010
N(4) – C(5)	1.336	1.333	0.010
C(5) – C(6)	1.475	1.473	0.011
C(6) – C(7)	1.390	1.389	0.012
C(7) – C(8)	1.372	1.372	0.013
C(8) – C(9)	1.410	1.408	0.016
C(9) – C(10)	1.370	1.368	0.013
C(10) – C(11)	1.385	1.383	0.012
C(11) – C(6)	1.413	1.410	0.013
C(2) – C(12)	1.515	1.513	0.011
C(12) – C(13)	1.388	1.387	0.011
C(13) – C(14)	1.396	1.396	0.015
C(14) – C(15)	1.360	1.360	0.017
C(15) – C(16)	1.385	1.385	0.015
C(16) – C(17)	1.393	1.391	0.013
C(17) – C(12)	1.417	1.415	0.012
Bond	l (Å)	Bond	l (Å)
C(7) – H(7)	0.89	C(13) – H(13)	1.13
C(8) – H(7)	1.01	C(14) – H(14)	0.88
C(9) – H(9)	1.07	C(15) – H(15)	1.05
C(10) – H(10)	1.07	C(16) – H(16)	0.96
C(11) – H(11)	0.94	C(17) – H(17)	1.10

Table 2. Bond angles ∠(ijk) in 2,5-diphenyl-3,4-diaza-6a-thiathiophthene. The standard deviations given in parentheses refer to the last digits of respective values.

i	j	k	∠(ijk)°	i	j	k	∠(ijk)°
C(2)	S(1)	S(6a)	91.3(3)	C(5)	C(6)	C(7)	122.6(8)
S(1)	S(6a)	S(6)	174.3(2)	C(5)	C(6)	C(11)	119.9(7)
S(1)	S(6a)	C(3a)	87.1(3)	C(7)	C(6)	C(11)	117.5(9)
S(6)	S(6a)	C(3a)	87.1(3)	C(6)	C(7)	C(8)	122.5(9)
S(6a)	S(6)	C(5)	91.9(3)	C(7)	C(8)	C(9)	118.6(9)
S(1)	C(2)	N(3)	122.2(6)	C(8)	C(9)	C(10)	120.2(9)
S(1)	C(2)	C(12)	121.2(6)	C(9)	C(10)	C(11)	120.6(9)
N(3)	C(2)	C(12)	116.6(7)	C(10)	C(11)	C(6)	120.5(8)
C(2)	N(3)	C(3a)	117.6(7)	C(2)	C(12)	C(13)	120.9(8)

Table 2. Continued.

N(3)	C(3a)	S(6a)	121.6(6)	C(2)	C(12)	C(17)	119.0(7)
N(3)	C(3a)	N(4)	116.8(8)	C(13)	C(12)	C(17)	120.0(8)
N(4)	C(3a)	S(6a)	121.5(6)	C(12)	C(13)	C(14)	118.5(9)
C(3a)	N(4)	C(5)	118.1(7)	C(13)	C(14)	C(15)	122.1(1.1)
N(4)	C(5)	S(6)	121.3(6)	C(14)	C(15)	C(16)	119.9(1.0)
N(4)	C(5)	C(6)	116.8(7)	C(15)	C(16)	C(17)	120.1(1.0)
C(6)	C(5)	S(6)	121.8(6)	C(16)	C(17)	C(12)	119.5(8)

Similarly, the twist angle of the 5-phenyl group about C(5) – C(6) was found to be 7.0°.

Comparison with the structure of 2,5-diphenyl-6a-thiathiophthene. Bond lengths in 2,5-diphenyl-6a-thiathiophthene (II) are given in Fig. 2.[5]

The sulphur-sulphur bonds are almost equal in the present structure where the 2- and 5-phenyl groups are twisted 2.0 and 7.0°, respectively; the bond lengths are S(1) – S(6a) = 2.319(3) Å and S(6a) – S(6) = 2.328(3) Å, *cf.* Fig. 1a.

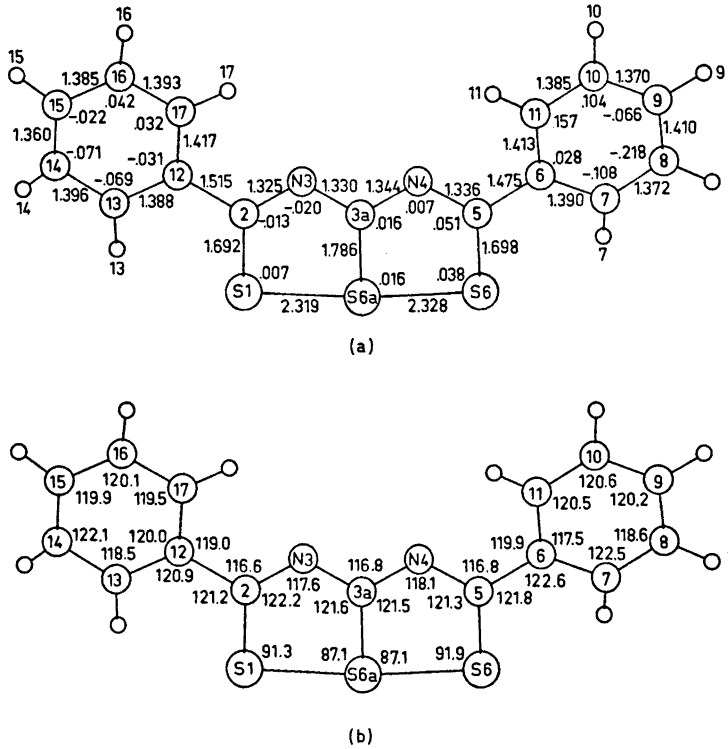


Fig. 1. (a) Bond lengths (Å) in 2,5-diphenyl-3,4-diaza-6a-thiathiophthene, and atomic distances (Å) from the least squares plane of the molecule. (b) Bond angles (°).

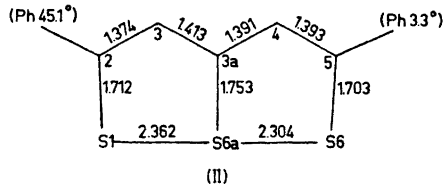


Fig. 2. Bond lengths (Å) in 2,5-diphenyl-6a-thiathiophthene.

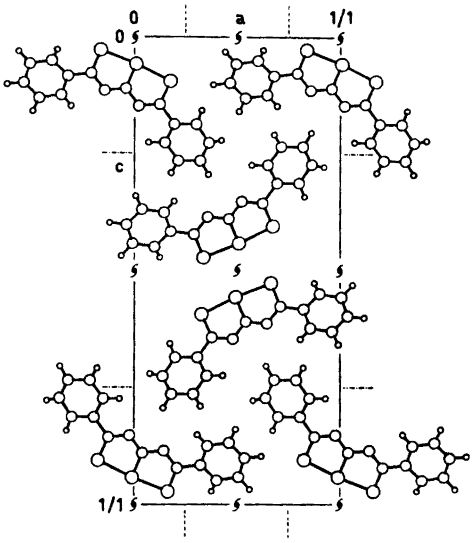


Fig. 3. The arrangement of 2,5-diphenyl-3,4-diaza-6a-thiathiophthene molecules in the crystal as seen along the *b*-axis.

In compound II, however, where the 2- and 5-phenyl groups are twisted 45.1 and 3.3° about the respective connecting bonds, the S – S bonds are significantly different, *i.e.* S(1) – S(6a) = 2.362(3) Å and S(6a) – S(6) = 2.304(3) Å. This agrees with the results from CNDO/2 calculations on phenyl substituted 6a-thiathiophthenes.[6] A 2-phenyl group will, according to the CNDO/2 results, cause a lengthening of the S(1) – S(6a) bond which varies with the twist angle of the phenyl group, being negligible at twist angle 0° and most pronounced at 90°.

The difference between the length of the S(6a) – C(3a) bond in I, 1.786(8) Å, and the length of the S(6a) – C(3a) bond in II, 1.753(6) Å, may be real, and due to the presence of the nitrogen atoms in I. Thus the S(6a) – C(3a) bond lengths in eleven different 6a-thiathiophthene structures are found in the range 1.748 – 1.763 Å,[7] while the S(6a) – C(3a) bond length in 2,5-dianilino-3,4-diaza-6a-thiathiophthene [8] is found to be 1.790(8) Å, in close agreement with the length of the equivalent bond in the present structure.

The lengths of the carbon-nitrogen bonds in I, C(2) – N(3) = 1.325(10) Å, N(3) – C(3a) = 1.330(9) Å, C(3a) – N(4) = 1.344(10) Å, and N(4) – C(5) = 1.336(10) Å, agree with the length of the aromatic C – N bond in pyridine, 1.340 Å,[9] and there is no significant difference between the central and the terminal C – N bond lengths. Also in this respect there seems to be a difference between 3,4-diaza-6a-thiathiophthenes and 6a-thiathiophthenes. The sum of the C(3a) – C(3) and the C(3a) – C(4) bond lengths in the latter is namely always found to be greater than the sum of the C(2) – C(3) and the C(4) – C(5) bond lengths.[7]

The crystal structure of 2,5-diphenyl-3,4-diaza-6a-thiathiophthene as seen along the *b*-axis is shown in Fig. 3. There are no intermolecular atomic distances shorter than the corresponding van der Waals distances.

EXPERIMENTAL

The unit cell dimensions for crystals of 2,5-diphenyl-3,4-diaza-6a-thiathiophthene were determined from high-order reflections on $0kl$ and $h0l$ Weissenberg photographs where lead nitrate powder lines had been superimposed for reference. A least squares procedure on 30 measured 2θ-values gave $a = 12.494(12)$ Å, $b = 4.007(8)$ Å, and $c = 28.185(15)$ Å.

Four molecules per unit cell give a calculated density of 1.480 g/cm³ as compared with the density 1.49 g/cm³ found by flotation.

The intensities of the $h0l - h3l$ reflections were estimated visually from Weissenberg photographs taken with Ni-filtered Cu$K\alpha$ radiation ($\mu = 45.2$ cm^{-1}).

A crystal with dimensions about $0.08 \times 0.7 \times 0.03$ mm in the three axial directions was used for the intensity data collection. Lp corrections, and corrections for extended spots on upper layer Weissenberg films, were applied, but absorption corrections were not applied.

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

Atom	*x*	*y*	*z*
S(1)	0.17397(15)	−0.0255(0)	0.09414(7)
S(6a)	0.00714(16)	−0.0127(11)	0.05747(6)
S(6)	−0.16457(18)	0.0279(9)	0.02732(6)
C(2)	0.12310(59)	0.1521(25)	0.14367(29)
N(3)	0.02089(45)	0.2338(21)	0.14743(20)
C(3a)	−0.04169(59)	0.1785(26)	0.11018(24)
N(4)	−0.14522(47)	0.2640(21)	0.11462(22)
C(5)	−0.20977(58)	0.2128(23)	0.07766(26)
C(6)	−0.32299(62)	0.3061(25)	0.08373(27)
C(7)	−0.41122(68)	0.2265(30)	0.05060(32)
C(8)	−0.50760(73)	0.2943(35)	0.05781(34)
C(9)	−0.53728(71)	0.4772(35)	0.09840(36)
C(10)	−0.46174(67)	0.5659(28)	0.13120(30)
C(11)	−0.35525(60)	0.4853(33)	0.12434(27)
C(12)	0.19300(53)	0.2230(23)	0.18632(28)
C(13)	0.30040(68)	0.1357(29)	0.18650(34)
C(14)	0.36122(97)	0.2101(45)	0.22665(38)
C(15)	0.31903(84)	0.3679(32)	0.26502(35)
C(16)	0.21237(79)	0.4620(40)	0.26485(32)
C(17)	0.14814(71)	0.3897(28)	0.22585(29)
H(7)	−0.3762(41)	0.100(17)	0.0271(18)
H(8)	−0.5624(58)	0.250(24)	0.0322(27)
H(9)	−0.5218(79)	0.512(47)	0.1002(36)
H(10)	0.4949(71)	0.710(33)	0.1596(34)
H(11)	0.3048(64)	0.522(40)	0.1484(33)
H(13)	0.3249(62)	0.025(39)	0.1556(32)
H(14)	0.4249(82)	0.119(43)	0.2220(46)
H(15)	0.3591(86)	0.480(61)	0.2937(43)
H(16)	0.1758(61)	0.562(32)	0.2910(29)
H(17)	0.0680(48)	0.522(29)	0.2259(21)

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

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
S(1)	941(10)	482(16)	454(9)	118(17)	−75(13)	103(8)
S(6a)	610(11)	299(12)	347(8)	38(13)	−29(12)	153(8)
S(6)	610(11)	475(17)	350(8)	−19(15)	−55(12)	58(8)
C(2)	430(43)	268(55)	539(45)	66(42)	82(42)	88(35)
N(3)	366(33)	381(50)	360(32)	55(34)	−39(33)	30(25)
C(3a)	461(44)	383(56)	325(35)	8(43)	23(39)	21(30)
N(4)	387(34)	440(52)	416(33)	50(35)	34(33)	29(26)
C(5)	488(42)	281(58)	368(38)	−16(43)	80(38)	57(33)
C(6)	458(43)	347(58)	436(41)	−18(45)	52(40)	−40(34)
C(7)	507(51)	487(70)	631(49)	35(49)	−1(50)	−57(40)
C(8)	526(52)	640(76)	651(56)	−8(58)	137(69)	−192(47)
C(9)	593(52)	458(69)	814(60)	44(82)	60(72)	94(48)
C(10)	483(45)	443(75)	553(46)	103(48)	−5(45)	77(36)
C(11)	508(44)	387(58)	491(40)	132(62)	3(53)	−32(33)
C(12)	388(42)	258(58)	432(40)	1(38)	72(37)	60(31)
C(13)	498(50)	535(74)	549(48)	130(47)	−123(50)	−5(39)
C(14)	752(77)	1062(117)	525(56)	−40(89)	−63(69)	−76(52)
C(15)	769(69)	664(94)	487(49)	−155(63)	91(52)	−161(48)
C(16)	688(56)	698(81)	513(45)	−11(76)	−215(64)	−4(41)
C(17)	514(49)	553(81)	490(46)	56(49)	−42(46)	−2(37)

	U		U
H(7)	130	H(13)	494
H(8)	161	H(14)	1072
H(9)	920	H(15)	707
H(10)	557	H(16)	441
H(11)	502	H(17)	99

The scattering factors used for sulphur, nitrogen, carbon and hydrogen in the structure factor calculations were those given in the *International Tables*.[10]

Final atomic coordinates from the least squares refinement are listed in Table 3, and the temperature parameters in Table 4. A pictorial representation of the thermal motion of the atoms is given in Fig. 4.[11]

An analysis of the thermal parameters of the S, N, and C atoms, assuming the whole molecule a rigid body, was carried out according to the method of Schomaker and True-

Table 5. Libration tensor L from the rigid-body analysis.

Eigenvalues		Eigenvectors (Direction cosines × 10^4 relative to *a*, *b*, and *c*, respectively)		
L	5.0 (°)^2	0.8408	0.4491	−0.3023
	3.1	0.0365	0.5017	0.8643
	2.9	0.5401	−0.7366	0.4070

Table 6. Observed and calculated structure factors for 2,5-diphenyl-3,4-diaza-6a-thia-thiophthene. The values given are ten times the absolute values. Unobserved reflections are marked with a minus sign in front of F_o.

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	2	6	1274	1321	3	0	14	421	418	6	0	11	-38	42	9	0	18	-47	0	13	0	12	-40	37
0	0	8	-23	21	3	0	15	611	604	6	0	12	-39	17	9	0	19	113	115	13	0	13	-39	25
0	2	10	227	229	3	0	16	149	148	6	0	13	-40	35	9	0	20	-46	41	13	0	14	-38	9
0	0	12	271	264	3	0	17	519	537	6	0	14	148	144	9	0	21	-45	20	13	0	15	-37	15
0	2	14	220	217	3	0	18	-41	30	6	0	15	-42	0	9	0	22	79	83	13	0	16	-35	5
0	0	16	210	205	3	0	19	401	315	6	0	16	192	186	9	0	23	-42	48	13	0	17	-33	10
0	2	18	-39	36	3	0	20	-44	35	6	0	17	-44	0	9	0	24	-41	17	13	0	18	-31	26
0	0	20	-42	31	3	0	21	74	70	6	0	18	68	66	9	0	25	-39	15	13	0	19	-29	12
0	2	22	164	166	3	0	22	-46	35	6	0	19	-46	4	9	0	26	-36	15	13	0	20	-26	35
0	0	24	432	453	3	0	23	-47	19	6	0	20	-47	12	9	0	27	-33	13	14	0	1	-40	40
0	2	26	141	135	3	0	24	-47	35	6	0	21	-47	26	9	0	28	-30	6	14	0	2	-40	37
0	0	28	206	215	3	0	25	-47	41	6	0	22	-47	35	9	0	29	-26	32	14	0	3	45	47
0	2	30	-44	16	3	0	26	-47	42	6	0	23	-47	52	10	0	1	-45	4	14	0	4	69	84
0	0	32	141	153	3	0	27	-47	9	6	0	24	157	216	10	0	2	-45	31	14	0	5	-39	15
0	2	34	237	238	3	0	28	-46	16	6	0	25	-46	2	10	0	3	140	141	14	0	6	-39	11
1	0	2	-14	15	3	0	29	113	112	6	0	26	170	164	10	0	4	90	85	14	0	7	38	68
1	0	3	37	38	3	0	30	-42	12	6	0	27	-43	48	10	0	5	-46	10	14	0	8	38	43
1	0	4	665	907	3	0	31	136	142	6	0	28	173	166	10	0	6	-46	19	14	0	9	73	91
1	0	5	87	83	3	0	32	-37	4	6	0	29	100	91	10	0	7	304	285	14	0	10	93	107
1	0	6	235	198	3	0	33	-34	40	6	0	30	-36	1	10	0	8	431	391	14	0	11	67	79
1	0	7	-22	21	3	0	34	-30	18	6	0	31	-33	41	10	0	9	458	442	14	0	12	48	78
1	0	8	498	481	4	0	1	142	133	6	0	32	157	163	10	0	10	204	188	14	0	13	36	44
1	0	9	138	132	4	0	2	204	215	7	0	1	342	403	10	0	11	71	43	14	0	14	34	49
1	0	10	716	707	4	0	3	206	204	7	0	2	196	208	10	0	12	58	71	14	0	15	-29	1
1	0	11	122	127	4	0	4	171	166	7	0	3	62	63	10	0	13	209	188	14	0	16	94	106
1	0	12	59	53	4	0	5	168	171	7	0	4	62	81	10	0	14	122	96	2	0	0	106	97
1	0	13	-31	31	4	0	6	103	106	7	0	6	-37	15	10	0	15	-47	2	4	0	0	126	121
1	0	14	-33	17	4	0	7	823	809	7	0	7	-38	15	10	0	15	-47	2	8	0	0	99	94
1	0	15	118	119	4	0	8	627	630	7	0	8	273	249	10	0	16	230	209	10	0	0	51	30
1	0	16	36	51	4	0	9	773	761	7	0	9	138	122	10	0	17	124	129	12	0	0	134	131
1	0	17	50	50	4	0	10	410	396	7	0	10	464	478	10	0	18	76	76	14	0	0	-41	41
1	0	18	239	319	4	0	11	49	49	7	0	11	263	242	10	0	19	89	78	0	1	4	717	783
1	0	19	148	152	4	0	12	125	127	7	0	12	-42	12	10	0	20	183	175	0	1	6	1028	1066
1	0	20	106	103	4	0	13	329	323	7	0	13	-43	55	10	0	21	-42	47	0	1	8	204	200
1	0	21	-44	37	4	0	14	235	246	7	0	14	43	59	10	0	22	104	92	0	1	10	53	39
1	0	22	314	303	4	0	15	-38	13	7	0	15	88	87	10	0	23	-39	45	0	1	12	127	131
1	0	23	332	352	4	0	16	456	455	7	0	16	99	110	10	0	24	60	65	0	1	14	304	297
1	0	24	448	473	4	0	17	272	274	7	0	17	-46	2	10	0	25	128	125	0	1	16	128	114
1	0	25	229	217	4	0	18	257	255	7	0	18	184	186	10	0	26	67	69	0	1	18	129	117
1	0	26	-47	39	4	0	19	183	155	7	0	19	58	67	10	0	27	73	76	0	1	20	54	88
1	0	27	-47	17	4	0	20	295	303	7	0	20	-47	8	11	0	2	134	136	0	1	22	324	303
1	0	28	-46	59	4	0	21	-44	16	7	0	21	79	87	11	0	3	-47	17	0	1	24	80	99
1	0	29	-45	27	4	0	22	-46	37	7	0	22	232	247	11	0	4	-47	1	0	1	26	216	205
1	0	30	44	69	4	0	23	186	200	7	0	23	113	122	11	0	5	-47	22	0	1	28	371	348
1	0	31	-41	9	4	0	24	115	124	7	0	24	225	236	11	0	6	82	65	0	1	30	231	224
1	0	32	127	126	4	0	25	243	212	7	0	25	114	129	11	0	7	71	53	0	1	32	218	209
1	0	33	152	143	4	0	26	141	127	7	0	26	-43	22	11	0	9	-47	38	0	1	34	95	99
1	0	34	132	139	4	0	27	86	94	7	0	27	61	73	11	0	10	-47	43	1	1	6	436	438
1	0	35	143	164	4	0	28	-45	38	7	0	28	-35	14	11	0	11	-47	6	1	1	7	251	234
2	0	1	384	357	4	0	29	-43	27	7	0	29	-36	30	11	0	12	-47	42	1	1	8	165	160
2	0	2	697	721	4	0	30	-41	35	7	0	30	57	77	11	0	13	-47	11	1	1	9	317	296
2	0	3	407	424	4	0	31	-38	33	8	0	1	72	85	11	0	14	92	101	1	1	10	427	418
2	0	4	595	585	4	0	32	-35	21	8	0	2	77	82	11	0	15	68	73	1	1	11	179	180
2	0	5	437	424	4	0	33	87	66	8	0	3	110	114	11	0	16	-45	57	1	1	12	223	218
2	0	6	54	61	5	0	1	706	718	8	0	4	-35	27	11	0	17	-44	15	1	1	13	116	107
2	0	7	363	348	5	0	2	82	72	8	0	5	196	209	11	0	18	-43	45	1	1	14	128	118
2	0	8	243	227	5	0	3	317	319	8	0	6	57	66	11	0	19	-41	27	1	1	15	162	162
2	0	9	356	371	5	0	4	355	352	8	0	7	162	154	11	0	20	-40	50	1	1	16	157	150
2	0	10	733	816	5	0	5	143	142	8	0	8	77	71	11	0	21	103	101	1	1	17	-44	53
2	0	11	499	508	5	0	6	212	216	8	0	9	322	300	11	0	22	87	62	1	1	18	-46	49
2	0	12	433	487	5	0	7	331	329	8	0	10	520	495	11	0	23	-33	9	1	1	19	-47	42
2	0	13	289	308	5	0	8	453	520	8	0	11	318	297	11	0	24	74	73	1	1	20	319	304
2	0	14	337	370	5	0	9	180	156	8	0	12	308	285	11	0	25	92	112	1	1	21	155	153
2	0	15	114	108	5	0	10	206	203	8	0	13	190	173	12	0	1	103	99	1	1	22	412	311
2	0	16	417	422	5	0	11	71	78	8	0	14	306	268	12	0	2	242	237	1	1	23	177	199
2	0	17	-38	32	5	0	12	183	190	8	0	15	147	159	12	0	3	202	204	1	1	24	218	199
2	0	18	494	543	5	0	13	38	55	8	0	16	254	245	12	0	4	88	110	1	1	25	202	169
2	0	19	257	262	5	0	14	124	128	8	0	17	71	99	12	0	5	-47	12	1	1	26	107	114
2	0	20	357	389	5	0	15	57	105	8	0	18	334	304	12	0	6	114	99	1	1	27	149	156
2	0	21	-44	31	5	0	16	73	93	8	0	19	-47	52	12	0	7	-47	14	1	1	28	-51	61
2	0	22	134	104	5	0	17	-43	0	8	0	20	91	99	12	0	8	119	116	1	1	29	262	247
2	0	23	341	333	5	0	18	119	119	8	0	21	-47	47	12	0	9	-46	36	1	1	30	47	65
2	0	24	139	104	5	0	19	143	131	8	0	22	46	60	12	0	10	56	43	1	1	31	180	164
2	0	25	371	333	5	0	20	127	132	8	0	23	123	116	12	0	11	-45	12	1	1	32	62	75
2	0	26	230	203	5	0	21	70	82	8	0	24	-44	23	12	0	12	-45	5	1	1	33	72	71
2	0	27	114	102	5	0	22	92	56	8	0	25	133	153	12	0	13	-44	3	1	1	34	49	53
2	0	28	-46	18	5	0	23	71	95	8	0	26	-40	41	12	0	14	48	61	2	1	1	160	158
2	0	29	-45	16	5	0	24	271	263	8	0	27	-38	53	12	0	15	-42	16	2	1	2	277	282
2	0	30	48	61	5	0	25	155	197	8	0	28	-35	31	12	0	16	99	100	2	1	3	166	164
2	0	31	-41	17	5	0	26	98	101	8	0	29	-32	4	12	0	17	-39	28	2	1	4	269	254
2	0	32	-38	14	5	0	27	138	127	8	0	30	56	61	12	0	18	-38	1	2	1	5	658	684
2	0	33	109	94	5	0	28	112	105	9	0	1	161	155	12	0	19	36	48	2	1	6	254	243
2	0	34	38	53	5	0	29	77	69	9	0	2	-42	43	12	0	20	34	45	2	1	7	274	251
2	0	35	79	81	5	0	30	55	55	9	0	3	121	108	12	0	21	39	58	2	1	8	322	315
3	0	1	621	598	5	0	31	40	48	9	0	4	106	102	12	0	22	-29	12	2	1	9	381	369
3	0	2	63	63	5	0	32	117	125	9	0	5	86	87	12	0	23	36	43	2	1	10	372	380
3	0	3	150	150	5	0	33	81	91	9	0	6	225	215	13	0	1	88	94	2	1	11	484	486
3	0	4	-23	25	6	0	1	79	80	9	0	7	-44	39	13	0	2	148	143	2	1	12	546	556
3	0	5	129	122	6	0	2	403	417	9	0	8	-44	6	13	0	3	78	86	2	1	13	272	277
3	0	6	207	154	6	0	3	102	101	9	0	9	289	265	13	0	4	80	94	2	1	14	521	545
3	0	7	94	79	6	0	4	126	127	9	0	11	138	128	13	0	5	-44	14	2	1	15	129	109
3	0	8	238	228	6	0	5	-33	15	9	0	12	447	461	13	0	6	114	129	2	1	16	192	186
3	0	9	641	647	6	0	6	368	375	9	0	13	139	126	13	0	7	-44	48	2	1	17	80	79
3	0	10	-29	28	6	0	7	-34	26	9	0	14	157	163	13	0	8	123	125	2	1	18	189	190
3	0	11	422	426	6	0	8	77	89	9	0	15	403	390	13	0	9	-43	32	2	1	19	345	323
3	0	12	533	522	6	0	9	85	75	9	0	16	71	82	13	0	10	91	101	2	1	20	397	383
3	0	13	173	186	6	0	10	-37	1	9	0	17	171	143	13	0	11	50	53	2	1	21	417	378

Table 6. 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)
2	1	22	228	213	5	1	27	95	105	9	1	8	-51	36	13	1	14	-40	36	3	2	1	173	163
2	1	23	136	117	5	1	28	47	59	9	1	9	58	68	13	1	15	-39	42	3	2	2	80	78
2	1	24	75	89	5	1	29	168	167	9	1	10	258	272	13	1	16	-37	34	3	2	3	166	155
2	1	25	60	65	5	1	30	59	62	9	1	11	327	292	13	1	17	-34	19	3	2	4	41	40
2	1	26	-53	43	5	1	31	138	142	9	1	12	65	91	13	1	18	-32	47	3	2	5	36	42
2	1	27	90	102	5	1	32	34	54	9	1	13	398	401	13	1	19	-28	25	3	2	6	141	141
2	1	28	62	82	5	1	33	-29	46	9	1	14	254	261	13	1	20	40	70	3	2	7	275	269
2	1	29	-49	26	6	1	1	171	175	9	1	15	246	236	14	1	1	-43	9	3	2	8	102	97
2	1	30	-47	39	6	1	2	418	462	9	1	16	242	211	14	1	2	-43	37	3	2	9	441	442
2	1	31	-44	39	6	1	3	93	102	9	1	17	-53	52	14	1	3	-43	30	3	2	10	-39	26
2	1	32	70	78	6	1	4	473	517	9	1	18	-52	54	14	1	4	-43	8	3	2	11	277	290
2	1	33	-36	11	6	1	5	132	135	9	1	19	192	180	14	1	5	76	66	3	2	12	80	85
2	1	34	48	62	6	1	6	348	379	9	1	20	-51	73	14	1	6	51	49	3	2	13	50	60
3	1	1	143	138	6	1	7	221	230	9	1	21	178	167	14	1	7	61	81	3	2	14	105	94
3	1	2	127	125	6	1	8	101	100	9	1	22	68	68	14	1	8	49	66	3	2	15	541	517
3	1	3	350	333	6	1	9	94	90	9	1	23	73	82	14	1	9	-39	36	3	2	16	214	202
3	1	4	64	63	6	1	10	-43	33	9	1	24	-44	10	14	1	10	68	47	3	2	17	717	654
3	1	5	194	184	6	1	11	-44	19	9	1	25	-41	45	14	1	11	-37	45	3	2	18	63	60
3	1	6	-29	22	6	1	12	167	163	9	1	26	-38	26	14	1	12	61	81	3	2	19	258	243
3	1	7	264	258	6	1	13	47	47	9	1	27	49	54	14	1	13	66	51	3	2	20	-53	76
3	1	8	178	171	6	1	14	150	155	9	1	28	-36	42	3	1	0	52	50	3	2	21	107	113
3	1	9	136	133	6	1	15	127	126	10	1	1	78	64	5	1	0	116	113	3	2	22	85	98
3	1	10	316	313	6	1	16	75	70	10	1	2	167	165	7	1	0	116	122	3	2	23	-53	78
3	1	11	528	525	6	1	17	62	64	10	1	3	165	146	9	1	0	69	54	3	2	24	-53	8
3	1	12	129	149	6	1	18	148	138	10	1	4	-52	14	11	1	0	155	168	3	2	25	-51	39
3	1	13	674	734	6	1	19	-53	67	10	1	5	215	190	13	1	0	60	74	3	2	26	-50	3
3	1	14	316	357	6	1	20	-53	40	10	1	6	64	93	0	2	2	407	489	3	2	27	-48	44
3	1	15	441	495	6	1	21	99	27	10	1	7	171	167	0	2	4	239	246	3	2	28	-45	7
3	1	16	214	206	6	1	22	149	149	10	1	8	118	106	0	2	6	563	561	3	2	29	73	78
3	1	17	85	91	6	1	23	-53	43	10	1	9	160	132	0	2	8	49	48	3	2	30	-39	25
3	1	18	146	134	6	1	24	109	85	10	1	10	182	177	0	2	10	47	42	3	2	31	66	87
3	1	19	366	369	6	1	25	-51	60	10	1	11	184	183	0	2	12	198	182	3	2	32	-29	24
3	1	20	97	96	6	1	26	85	98	10	1	12	165	162	0	2	14	201	193	4	2	1	208	216
3	1	21	316	309	6	1	27	-47	64	10	1	13	-53	17	0	2	16	204	192	4	2	2	114	118
3	1	22	-52	23	6	1	28	209	223	10	1	14	188	166	0	2	18	195	193	4	2	3	222	226
3	1	23	233	230	6	1	29	-42	46	10	1	15	-53	35	0	2	20	-52	59	4	2	4	126	121
3	1	24	-53	20	6	1	30	173	193	10	1	16	151	134	0	2	22	93	90	4	2	5	113	114
3	1	25	70	66	6	1	31	83	87	10	1	17	117	116	0	2	24	118	106	4	2	6	227	250
3	1	26	-53	9	6	1	32	106	128	10	1	18	61	65	0	2	26	372	355	4	2	7	462	489
3	1	27	82	99	7	1	1	206	215	10	1	19	73	83	0	2	28	224	225	4	2	8	168	183
3	1	28	-50	43	7	1	2	138	138	10	1	20	100	104	0	2	30	205	199	4	2	9	225	227
3	1	29	72	81	7	1	3	293	329	10	1	21	122	121	0	2	32	181	215	4	2	10	247	248
3	1	30	-46	29	7	1	4	347	356	10	1	22	111	116	1	2	1	326	379	4	2	11	113	130
3	1	31	-47	49	7	1	5	330	342	10	1	23	142	149	1	2	2	208	231	4	2	12	100	106
3	1	32	-39	11	7	1	6	261	277	10	1	24	122	121	1	2	3	585	649	4	2	13	90	94
3	1	33	-35	31	7	1	7	201	203	10	1	25	43	58	1	2	4	491	504	4	2	14	76	76
3	1	34	-30	28	7	1	8	187	192	10	1	26	44	50	1	2	5	202	187	4	2	15	140	127
4	1	1	239	236	7	1	9	220	213	11	1	1	142	131	1	2	6	349	349	4	2	16	308	272
4	1	2	80	87	7	1	10	220	213	11	1	2	65	72	1	2	7	609	604	4	2	17	196	195
4	1	3	331	322	7	1	11	94	109	11	1	3	211	186	1	2	8	557	566	4	2	18	356	328
4	1	4	84	82	7	1	12	171	164	11	1	4	173	150	1	2	9	450	442	4	2	19	166	146
4	1	5	468	450	7	1	13	78	88	11	1	5	230	228	1	2	10	457	424	4	2	20	152	148
4	1	6	190	191	7	1	14	57	57	11	1	6	146	156	1	2	11	170	167	4	2	21	76	88
4	1	7	110	113	7	1	15	116	119	11	1	7	80	83	1	2	12	115	111	4	2	22	-53	51
4	1	8	131	125	7	1	16	158	153	11	1	8	-53	47	1	2	13	42	26	4	2	23	136	138
4	1	9	264	255	7	1	17	-52	57	11	1	9	-53	60	1	2	14	107	103	4	2	24	78	91
4	1	10	329	351	7	1	18	65	63	11	1	10	128	118	1	2	15	-45	23	4	2	25	166	157
4	1	11	248	255	7	1	19	-53	24	11	1	11	-53	44	1	2	16	-47	51	4	2	26	96	98
4	1	12	387	411	7	1	20	178	172	11	1	12	103	114	1	2	17	145	141	4	2	27	117	105
4	1	13	96	99	7	1	21	59	70	11	1	13	63	76	1	2	18	236	229	4	2	28	110	90
4	1	14	366	382	7	1	22	182	177	11	1	14	-51	9	1	2	19	125	119	4	2	29	49	63
4	1	15	-44	35	7	1	23	-52	61	11	1	15	-50	47	1	2	20	101	108	4	2	30	-36	31
4	1	16	277	268	7	1	24	-50	55	11	1	16	-45	35	1	2	21	75	59	4	2	31	55	62
4	1	17	93	76	7	1	25	-49	60	11	1	17	65	86	1	2	22	80	83	5	2	1	317	328
4	1	18	203	192	7	1	26	104	107	11	1	18	-46	49	1	2	23	-54	61	5	2	2	141	124
4	1	19	221	199	7	1	27	-44	45	11	1	19	-44	31	1	2	24	176	162	5	2	3	300	308
4	1	20	245	247	7	1	28	71	77	11	1	20	67	77	1	2	25	184	189	5	2	4	55	65
4	1	21	267	271	7	1	29	137	138	11	1	21	49	54	1	2	26	158	156	5	2	6	323	340
4	1	22	208	191	7	1	30	-34	16	11	1	22	74	95	1	2	27	222	224	5	2	7	173	196
4	1	23	157	185	7	1	31	106	134	11	1	23	99	109	1	2	28	82	94	5	2	8	228	240
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4	1	27	62	79	8	1	4	-46	55	12	1	3	-52	56	1	2	32	-33	35	5	2	12	103	100
4	1	28	-49	54	8	1	5	252	273	12	1	4	207	210	2	2	1	236	245	5	2	13	91	73
4	1	29	-47	8	8	1	6	142	126	12	1	5	78	83	2	2	2	175	166	5	2	14	136	135
4	1	30	-44	59	8	1	7	250	236	12	1	6	64	72	2	2	3	117	119	5	2	15	-51	48
4	1	31	-41	19	8	1	8	201	194	12	1	7	63	68	2	2	4	117	117	5	2	16	-52	2
4	1	32	-37	42	8	1	9	163	152	12	1	8	-51	56	2	2	5	242	243	5	2	17	-53	48
4	1	33	-32	38	8	1	10	250	225	12	1	9	-51	4	2	2	6	246	226	5	2	18	146	137
5	1	1	254	266	8	1	11	322	294	12	1	10	-50	37	2	2	7	643	658	5	2	19	153	146
5	1	2	300	304	8	1	12	405	381	12	1	11	-50	24	2	2	8	516	500	5	2	20	66	83
5	1	3	678	711	8	1	13	266	249	12	1	12	54	75	2	2	9	303	296	5	2	21	80	86
5	1	4	609	645	8	1	14	258	263	12	1	13	-48	5	2	2	10	84	93	5	2	22	-53	65
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5	1	7	131	130	8	1	17	92	101	12	1	16	-44	2	2	2	13	174	177	5	2	25	177	175
5	1	8	92	89	8	1	18	-53	58	12	1	17	-42	16	2	2	14	161	155	5	2	26	138	147
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5	1	16	-48	37	8	1	26	-43	24	13	1	3	69	60	2	2	22	-54	61	6	2	4	105	105
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5	1	25	90	92	9	1	6	-50	53	13	1	12	71	88	2	2	31	-36	49	6	2	13	-51	45
5	1	26	-51	45	9	1	7	203	174	13	1	13	-42	34	2	2	32	44	48	6	2	14	118	128

Table 6. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
6	2	15	-52	20	9	2	25	39	31	0	3	26	-44	46	4	3	7	168	183	7	3	21	61	64
6	2	16	131	121	10	2	1	-54	30	0	3	28	169	195	4	3	8	158	152	7	3	22	-40	34
6	2	17	-53	26	10	2	2	-54	61	1	3	1	103	122	4	3	9	-50	53	7	3	23	-36	16
6	2	18	76	88	10	2	3	122	117	1	3	2	84	87	4	3	10	84	91	8	3	1	103	97
6	2	19	-54	27	10	2	4	-54	17	1	3	3	266	293	4	3	11	209	202	8	3	2	-55	33
6	2	20	80	76	10	2	5	164	151	1	3	4	180	194	4	3	12	364	337	8	3	3	-55	44
6	2	21	59	68	10	2	6	93	89	1	3	5	291	314	4	3	13	243	226	8	3	4	-55	57
6	2	22	63	77	10	2	7	165	145	1	3	6	292	298	4	3	14	260	248	8	3	5	158	153
6	2	23	-50	19	10	2	8	-53	45	1	3	7	153	151	4	3	15	82	89	8	3	6	149	167
6	2	24	68	62	10	2	9	93	92	1	3	8	-40	21	4	3	16	139	120	8	3	7	160	153
6	2	25	-46	56	10	2	10	-53	66	1	3	9	108	113	4	3	17	95	80	8	3	8	82	84
6	2	26	207	215	10	2	11	-52	31	1	3	10	114	120	4	3	18	91	87	8	3	9	-55	16
6	2	27	74	69	10	2	12	-52	48	1	3	11	-47	39	4	3	19	66	49	8	3	10	77	74
6	2	28	128	133	10	2	13	96	94	1	3	12	95	90	4	3	20	122	117	8	3	11	81	98
6	2	29	76	82	10	2	14	-50	8	1	3	13	80	83	4	3	21	186	177	8	3	12	136	113
7	2	1	261	250	10	2	15	110	104	1	3	14	140	132	4	3	22	166	161	8	3	13	91	90
7	2	2	195	194	10	2	16	72	66	1	3	15	112	104	4	3	23	148	126	8	3	14	210	199
7	2	3	236	232	10	2	17	125	119	1	3	16	76	86	4	3	24	106	105	8	3	15	-51	14
7	2	4	210	223	10	2	18	186	175	1	3	17	-55	53	4	3	25	63	72	8	3	16	128	125
7	2	5	103	111	10	2	19	183	183	1	3	18	137	144	4	3	26	54	70	8	3	17	170	159
7	2	6	238	229	10	2	20	98	95	1	3	19	-55	51	4	3	27	41	55	8	3	18	109	98
7	2	7	367	358	10	2	21	-39	8	1	3	20	106	108	5	3	1	127	145	8	3	19	120	121
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7	2	9	246	228	10	2	23	97	93	1	3	22	91	77	5	3	3	225	240	8	3	21	84	89
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7	2	17	66	70	11	2	8	85	84	2	3	2	41	48	5	3	11	-54	76	9	3	7	113	97
7	2	18	56	114	11	2	9	-51	12	2	3	3	110	111	5	3	12	98	104	9	3	8	-53	70
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8	2	19	77	99	12	2	17	-34	25	3	3	4	64	65	6	3	15	-55	27	10	3	16	71	82
8	2	20	-50	53	12	2	18	-31	27	3	3	5	146	149	6	3	16	-54	36	11	3	1	-48	41
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9	2	18	127	114	0	3	12	129	138	3	3	28	-31	19	7	3	14	66	83	12	3	10	-31	49
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9	2	20	89	100	0	3	16	81	87	4	3	2	82	91	7	3	16	-52	65	3	3	0	36	31
9	2	21	97	78	0	3	18	83	88	4	3	3	132	130	7	3	17	-51	41	5	3	0	133	148
9	2	22	-42	49	0	3	20	-55	40	4	3	4	73	86	7	3	18	99	93	7	3	0	140	131
9	2	23	-39	31	0	3	22	121	123	4	3	5	159	160	7	3	19	72	77	9	3	0	-55	30
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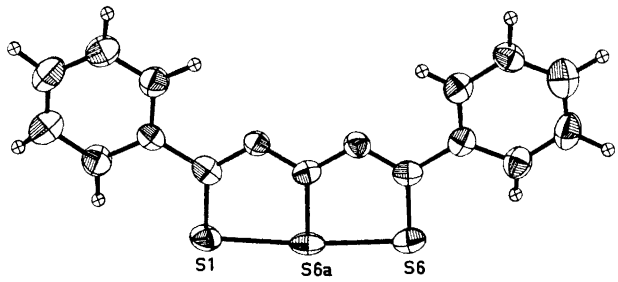

Fig. 4. The thermal ellipsoid plot showing the anisotropic vibration of the non-hydrogen atoms.

blood.[3] The libration tensor **L** arrived at is given in Table 5. Bond lengths, which have been corrected according to the libration tensor L, are listed in the first column of Table 1.

The final list of structure factors is given in Table 6.

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