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The Crystal and Molecular Structure of 2,4-Diphenyl-dithiofurophthene

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An X-ray structure study of crystals of 2,4-diphenyl-dithiofurophthene has been carried out. The crystals belong to the space group *Pbca*, with unit cell dimensions: $a = 14.28$ Å, $b = 27.77$ Å and $c = 7.186$ Å. There are eight molecules per unit cell.

The structure was solved by three-dimensional Patterson synthesis, and the parameters were refined by least squares methods. The refinement comprises the *hk*0-*hk*5 and 0*kl* reflections.

The dithiofurophthene system is almost planar, and the lengths of the different bonds there are, $S_1-S_2 = 2.106(3)$, $S_2-O = 2.382(6)$, $S_1-C_1 = 1.705(7)$, $S_2-C_3 = 1.757(7)$, $O-C_5 = 1.260(10)$, $C_1-C_2 = 1.354(10)$, $C_2-C_3 = 1.420(10)$, $C_3-C_4 = 1.389(10)$, and $C_4-C_5 = 1.428(10)$ Å, with the standard deviations given in the brackets. The S_1-S_2-O angle is $174.7 \pm 0.2°$.

The bonds which connect the phenyl groups to the dithiofurophthene system are, $C_1-C_6 = 1.482(10)$, Å and $C_4-C_{12} = 1.480(10)$ Å.

The plane of the phenyl group bonded to C_1, and the plane of that bonded to C_4 form angles of 24.3° and 119.6°, respectively, with the plane of the disulphide ring.

The thiothiophthene "no-bond resonance" system with equally spaced and partially bonded sulphur atoms in a linear sulphur sequence, was discovered ten years ago by Bezzi *et al.*[1-3] through an X-ray crystallographic study of the symmetric dimethyl derivative, compound (I). The term "no-bond resonance" followed the valence-bond description of this molecular system, as resonance forms such as (II) and (III) had to be taken into account.

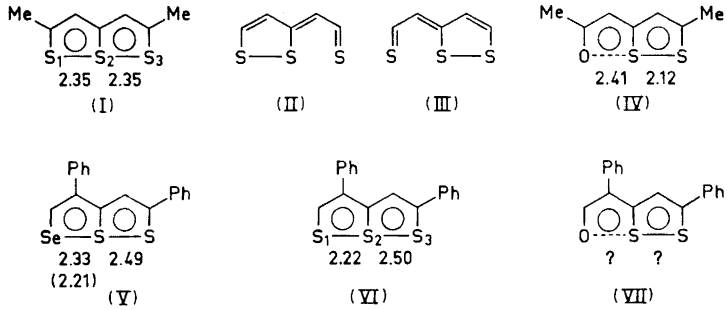
However, it may be quite as convenient to describe and probably also understand the bonding in compounds of the thiothiophthene type in terms of available molecular-orbital theories. According to those the thiothiophthene system may be described as follows:

1. There is a delocalized σ-system in the sulphur sequence, equivalent to that in trihalide ions and referred to as a three-center four-electron bond.

2. There is in addition a delocalized π-system composed of the 10 electrons in p-orbitals perpendicular to the plane of the two fused rings.

Hence the partial bonds in the linear sequence are both σ and π in character, but they are weaker than the other bonds in the molecule and therefore more liable to changes in bond length when the σ-system or the π-system is perturbed to some degree.

The results from the structure analysis of compound (IV) by Mammi *et al.*[4] show that if one of the terminal sulphur atoms in (I) is replaced by an oxygen atom, the remaining sulphur-sulphur bond shrinks to 2.12 Å which is close to the value 2.10 Å for a sulphur-sulphur single bond in a *cis* planar disulphide group.[5] The O—S distance 2.41 Å is 0.8 Å shorter than the corresponding van der Waals distance and 0.7 Å longer than the sum of covalent single-bond radii for oxygen and sulphur.



The structure of compound (VI) has been studied by the authors.[6] The sulphur-sulphur bonds there are different, 2.22 and 2.50 Å, respectively. As the phenyl-substituents in this compound are in unsymmetrical positions it seems likely that the bonding in the thiothiophthene system is perturbed in an unsymmetrical way, and this may explain why the two sulphur-sulphur bond lengths are different.

In compound (V) which is analogous to (VI) there is a selenium-sulphur-sulphur sequence. The structure of this compound has been studied by van den Hende and Klingsberg.[7] They found the selenium-sulphur bond length to be 2.33 Å and the sulphur-sulphur bond length 2.49 Å. If the difference in covalent radii between selenium and sulphur is subtracted from the found selenium-sulphur bond length one gets the value 2.21 Å. This shows that the bonding in the selenium-sulphur-sulphur sequence of compound (V) is practically the same as the bonding in the tri-sulphur sequence of compound (VI), that is, *one* of the bonds in the sequence is stronger than the other one.

The question is now, do the phenyl groups in compound (VII) cause a similar shortening of the O—S bond there relative to the O—S bond in compound (IV).

STRUCTURE DETERMINATION

Crystals of compound (VII) were generously supplied by Klingsberg. The crystals are orange by colour and belong to the orthorhombic space group *Pbca*. For cell dimensions, see EXPERIMENTAL.

The structure analysis is based on photographic data, taken with Weissenberg camera and Cu$K\alpha$ radiation. The data comprises 1350 observed $hk0$-$hk5$ and $0kl$ reflections.

Approximate coordinates for the sulphur atoms, the oxygen atom, and the carbon atoms of the five-membered rings were found from a three-dimensional Patterson map, and the orientation of the phenyl groups relative to the plane of the five-membered rings could be roughly estimated from packing considerations. The trial structure thus arrived at refined rapidly.

The calculations were carried out on an IBM 1620[II] computer, using a block-diagonal least squares program designed by Mair.[8] Anisotropic temperature factors were applied to sulphur, oxygen, and carbon, and isotropic temperature factors were applied to hydrogen. The final R factor is 7.9 %.

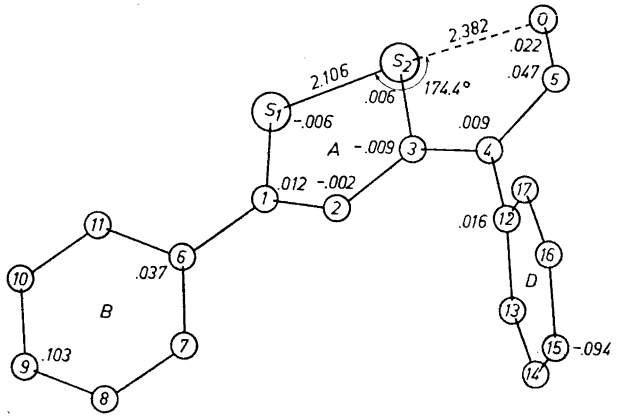


Fig. 1. The 2,4-diphenyl-dithiofurophthene molecule as seen along the c axis. Bond lengths and deviations from the plane of ring A in Å units.

DISCUSSION

Fig. 1 shows the molecule as seen along the c axis. The S_1—S_2 distance is 2.106±0.003 Å and the S_2—O distance 2.382±0.006 Å. The S_1—S_2—O angle is 174.4±0.2° and the sulphur-sulphur-oxygen sequence is thus almost linear.

The disulphide ring A is planar within the error and the atoms C_4, C_5, and O lie close to this plane. With regard to the carbon atoms of the phenyl groups B and D and their respective least squares planes, there is no deviation greater than 0.01 Å. The normal to the plane of A forms angles of 24.3 and 119.6° respectively, with the normals to the planes of B and D.

The carbon sequence C_1—C_6—C_9 which is almost linear, forms a small angle with the plane of ring A. Thus C_6 and C_9 lie out of this plane by 0.04 and 0.10 Å, respectively.

The sequence C_4—C_{12}—C_{15} shows a small but significant deviation from linearity which probably may be noticed from the figure. C_4 lies 0.10 Å out

from the plane of ring D, and the bond $C_{12}-C_4$ forms an angle of 3.7° with this plane. Hence the phenyl group D seems to be slightly bent about C_{12}. For further structural details, see RESULTS.

Fig. 2 shows the arrangement of the eight molecules of a unit cell, viewed along c. The indicated symmetry elements are those which follow from the three mutually perpendicular glide planes.

A contact of 3.35 Å between S_1 of $A1$ and C_{11} of $B2$ gives rise to helices of molecules about the c screw axes. These helices are held together by van der

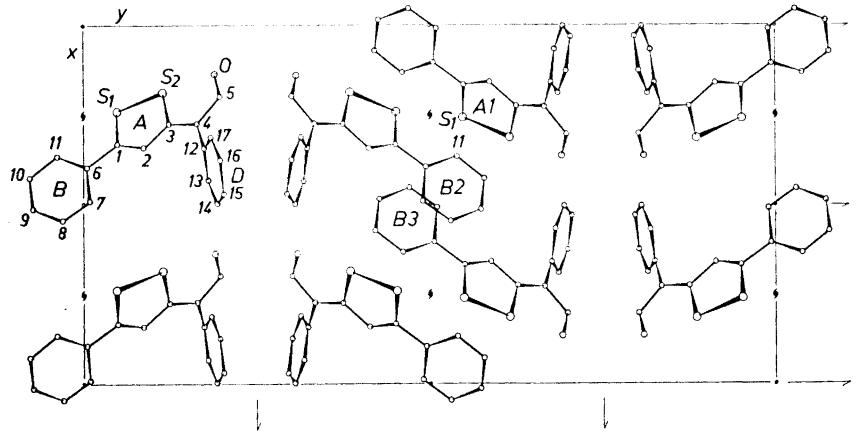


Fig. 2. The arrangement of the eight molecules of the unit cell viewed along c.

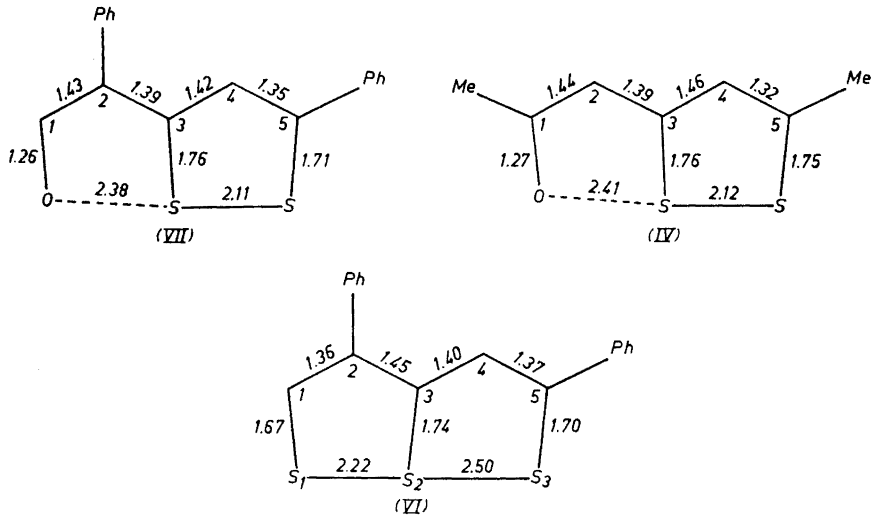


Fig. 3. Comparison of bond lengths (Å) in 2,4-diphenyl-dithiofurophthene (VII) with bond lengths in 2,5-dimethyl-dithiofurophthene (IV) and 2,4-diphenyl-thiothiophthene (VI).

Waals interaction between the phenyl groups $B2$ and $B3$. The latter are arranged over centres of symmetry, they are thus parallel, and they cover each other to about 60 % at a distance of 3.42 Å. The contacts across the glide plane perpendicular to the b axis are less pronounced. This probably explains why the compound tends to crystallize as flakes with (010) as the predominant face.

A comparison of bond lengths is given in Fig. 3. The O—S distance in the present compound is 2.38 Å as compared with the O—S distance of 2.41 Å in the symmetric dimethyl derivative. The difference in O—S distance is hardly significant, but in the direction one should expect. The other bond lengths in the molecules (VII) and (IV) agree within the error, and the alternating short and long bonds in the carbon part of the dithiofurophthene system seems to be a significant feature in this molecular system.

The variation of C—C bond lengths in the carbon part of the sulphur analog, compound (VI), is different. As regards the ring to the left the sequence of short and long bonds is reversed, but this agrees with the results from the structure study of the selenium analog.[7]

Table 1. Atomic coordinates in fractions of corresponding cell edges.

Atom	x	y	z
S(1)	0.24157	0.04913	0.03592
S(2)	0.18688	0.11574	0.12435
O	0.13685	0.19128	0.24577
C(1)	0.33187	0.04807	0.19118
C(2)	0.33981	0.08658	0.30569
C(3)	0.27377	0.12467	0.29400
C(4)	0.27205	0.16558	0.40508
C(5)	0.19661	0.19825	0.37196
C(6)	0.39538	0.00586	0.19120
C(7)	0.48472	0.00894	0.26122
C(8)	0.54490	-0.03086	0.26061
C(9)	0.51446	-0.07408	0.19308
C(10)	0.42538	-0.07851	0.12438
C(11)	0.36638	-0.03907	0.12347
C(12)	0.34074	0.17655	0.55339
C(13)	0.43539	0.18164	0.50773
C(14)	0.49947	0.19470	0.65001
C(15)	0.47047	0.20386	0.82601
C(16)	0.37521	0.19865	0.87030
C(17)	0.31032	0.18521	0.73463
H(2)	0.3877	0.0840	0.3932
H(5)	0.1907	0.2281	0.4504
H(7)	0.5144	0.0364	0.3165
H(8)	0.5992	-0.0293	0.3223
H(9)	0.5567	-0.0996	0.1678
H(10)	0.4247	-0.1112	0.0996
H(11)	0.3222	-0.0365	0.0896
H(13)	0.4495	0.1758	0.3568
H(14)	0.5660	0.1962	0.6066
H(15)	0.5200	0.2085	0.9268
H(16)	0.3544	0.2056	0.9752
H(17)	0.2366	0.1812	0.7677

EXPERIMENTAL

The unit cell dimensions for crystals of 2,4-diphenyl-dithiofurophthene were determined from high order axial reflections on Weissenberg photographs. The cell dimensions found in this way, $a = 14.28$, $b = 27.77$, and $c = 7.186$ Å, are believed to be within ± 0.2 % of the correct values. Eight molecules per unit cell give a calculated density of 1.382 g/cm^3 as compared with the density 1.38 g/cm^3 found by flotation.

The intensities of the $hk0$-$hk5$ and $0kl$ reflections were estimated visually from Weissenberg photographs taken with copper radiation (Cu$K\alpha$). Small crystals were used in order to minimize absorption effects, and no absorption correction was applied. The intensities were corrected in the usual way to give sets of relative structure factors. Common reflections in $hk0$-$hk5$ and $0kl$ were used to put all the reflections on the same scale.

The calculated structure factors were based on the atomic scattering curves for sulphur, oxygen, carbon, and hydrogen given in the *International Tables*, the first set of the listed scattering factors for carbon being used.

Weighting scheme No. 3, recommended by Mair,[8] was used in the least squares refinement. F_{min} was taken as 2.5. The different layers of reflections were rescaled at the end of the isotropic refinement.

Some low order reflections, supposed to be affected by secondary extinction, were excluded from the least squares refinement, Unobserved reflections were excluded in order to save computer time.

The least squares refinement comprises 1311 observed reflections, and the final F_o and F_c values for these are listed in Table 5.

Table 2. Temperature parameters β_{ij} for sulphur, oxygen and carbon, and B for hydrogen. The expressions used are $\exp-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+kl\beta_{23}+hl\beta_{13})$ for sulphur, oxygen, and carbon, and $\exp-[B(\sin^2\theta/\lambda^2)]$ for hydrogen.

	β_{11}	β_{22}	β_{33}	β_{23}	β_{13}	β_{12}
S(1)	0.0078	0.0022	0.0271	−0.0020	−0.0050	−0.0007
S(2)	0.0067	0.0023	0.0289	0.0010	−0.0052	0.0002
O	0.0076	0.0026	0.0446	−0.0002	−0.0090	0.0019
C(1)	0.0076	0.0016	0.0194	−0.0001	0.0013	−0.0014
C(2)	0.0064	0.0018	0.0226	0.0010	−0.0013	−0.0003
C(3)	0.0060	0.0017	0.0272	0.0014	0.0002	−0.0004
C(4)	0.0062	0.0016	0.0280	0.0012	−0.0002	−0.0001
C(5)	0.0076	0.0021	0.0360	−0.0001	−0.0017	0.0016
C(6)	0.0070	0.0016	0.0201	0.0003	0.0015	−0.0014
C(7)	0.0072	0.0016	0.0245	−0.0010	−0.0017	−0.0008
C(8)	0.0076	0.0018	0.0287	0.0005	−0.0002	0.0001
C(9)	0.0106	0.0016	0.0259	0.0008	0.0046	0.0002
C(10)	0.0104	0.0015	0.0299	−0.0011	0.0053	−0.0006
C(11)	0.0093	0.0020	0.0234	−0.0006	−0.0029	−0.0015
C(12)	0.0057	0.0013	0.0282	0.0010	−0.0010	0.0006
C(13)	0.0065	0.0013	0.0320	0.0015	−0.0018	−0.0002
C(14)	0.0066	0.0015	0.0414	−0.0004	−0.0003	0.0001
C(15)	0.0076	0.0016	0.0401	−0.0037	−0.0072	0.0006
C(16)	0.0098	0.0020	0.0295	−0.0027	0.0003	0.0011
C(17)	0.0070	0.0017	0.0320	−0.0008	−0.0000	0.0001

	B (Å^2)		B(Å^2)		B (Å^2)
H(2)	2.8	H(9)	4.5	H(14)	1.9
H(5)	5.4	H(10)	6.2	H(15)	3.6
H(7)	1.9	H(11)	4.2	H(16)	3.6
H(8)	2.1	H(13)	3.4	H(17)	2.6

Table 3. Bond lengths D(ij) in 2,4-diphenyl-dithiofurophthene. The standard deviations given in parentheses refer to the last digits of respective values. For bonds including a hydrogen atom the standard deviation in bond length is estimated to be 0.08 Å.

i	j	D(ij)	i	j	D(ij)
S(1)	S(2)	2.106(3) Å	C(13)	C(14)	1.419(11) Å
S(1)	C(1)	1.705(7)	C(14)	C(15)	1.355(12)
S(2)	C(3)	1.757(7)	C(15)	C(16)	1.405(11)
S(2)	O	2.382(6)	C(16)	C(17)	1.396(12)
O	C(5)	1.260(10)	C(17)	C(12)	1.394(11)
C(1)	C(2)	1.354(10)	C(2)	H(2)	0.93
C(1)	C(6)	1.482(10)	C(5)	H(5)	1.01
C(2)	C(3)	1.420(10)	C(7)	H(7)	0.96
C(3)	C(4)	1.389(10)	C(8)	H(8)	0.89
C(4)	C(5)	1.428(10)	C(9)	H(9)	0.95
C(4)	C(12)	1.480(10)	C(10)	H(10)	0.93
C(6)	C(7)	1.374(10)	C(11)	H(11)	0.68
C(7)	C(8)	1.400(10)	C(13)	H(13)	1.12
C(8)	C(9)	1.366(11)	C(14)	H(14)	1.00
C(9)	C(10)	1.370(12)	C(15)	H(15)	1.02
C(10)	C(11)	1.382(11)	C(16)	H(16)	0.83
C(11)	C(6)	1.402(10)	C(17)	H(17)	1.09
C(12)	C(13)	1.398(9)			

Table 4. Bond angles ∠(ijk) in 2,4-diphenyl-dithiofurophthene. The standard deviations given in parentheses refer to the last digits of respective values. For bond angles including a hydrogen atom the standard deviation is estimated to be 5°.

i	j	k	∠(ijk)	i	j	k	∠(ijk)
C(1)	S(1)	S(2)	95.6(3)	C(13)	C(14)	C(15)	121.6(7)
S(1)	S(2)	C(3)	94.1(3)	C(14)	C(15)	C(16)	119.2(7)
S(1)	S(2)	O	174.4(2)	C(15)	C(16)	C(17)	120.8(8)
C(3)	S(2)	O	80.4(3)	C(16)	C(17)	C(12)	119.5(7)
S(2)	O	C(5)	101.3(5)	H(2)	C(2)	C(1)	114
S(1)	C(1)	C(2)	116.6(5)	H(2)	C(2)	C(3)	126
S(1)	C(1)	C(6)	118.5(5)	H(5)	C(5)	O	118
C(2)	C(1)	C(6)	125.0(6)	H(5)	C(5)	C(4)	120
C(1)	C(2)	C(3)	119.8(6)	H(7)	C(7)	C(6)	128
C(2)	C(3)	S(2)	113.9(5)	H(7)	C(7)	C(8)	111
C(2)	C(3)	C(4)	112.1(5)	H(8)	C(8)	C(7)	119
C(4)	C(3)	S(2)	120.1(5)	H(8)	C(8)	C(9)	120
C(3)	C(4)	C(5)	115.9(7)	H(9)	C(9)	C(8)	122
C(3)	C(4)	C(12)	124.8(6)	H(9)	C(9)	C(10)	117
C(5)	C(4)	C(12)	119.3(7)	H(10)	C(10)	C(9)	100
C(4)	C(5)	O	122.2(7)	H(10)	C(10)	C(11)	140
C(1)	C(6)	C(7)	121.3(6)	H(11)	C(11)	C(10)	131
C(1)	C(6)	C(11)	121.5(6)	H(11)	C(11)	C(6)	108
C(7)	C(6)	C(11)	117.2(6)	H(13)	C(13)	C(12)	113
C(6)	C(7)	C(8)	121.3(6)	H(13)	C(13)	C(14)	128
C(7)	C(8)	C(9)	120.0(7)	H(14)	C(14)	C(13)	113
C(8)	C(9)	C(10)	120.2(7)	H(14)	C(14)	C(15)	125
C(9)	C(10)	C(11)	119.8(7)	H(15)	C(15)	C(14)	118
C(10)	C(11)	C(6)	121.6(7)	H(15)	C(15)	C(16)	122
C(4)	C(12)	C(13)	119.5(7)	H(16)	C(16)	C(15)	122
C(4)	C(12)	C(17)	120.1(6)	H(16)	C(16)	C(17)	117
C(13)	C(12)	C(17)	120.2(7)	H(17)	C(17)	C(16)	121
C(12)	C(13)	C(14)	118.7(7)	H(17)	C(17)	C(12)	119

Table 5. Observed and calculated structure factors for 2,4-diphenyl-dithiofurophthene. The values are five times the absolute values.

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	0	0	392	390	8	6	0	100	112	1	18	1	97	118	6	1	1	249	- 267
6	0	0	354	376	8	7	0	125	132	1	19	1	49	- 57	6	2	1	114	- 108
8	0	0	77	66	8	8	0	209	- 240	1	20	1	103	- 104	6	3	1	209	- 184
10	0	0	57	- 61	8	9	0	121	- 130	1	22	1	109	- 126	6	4	1	294	- 260
12	0	0	82	106	8	10	0	181	- 174	1	25	1	64	- 69	6	5	1	68	64
14	0	0	74	- 67	8	11	0	37	- 47	1	26	1	58	- 68	6	6	1	135	132
16	0	0	66	66	8	13	0	37	- 47	1	28	1	72	- 71	6	7	1	65	59
0	10	0	665	708	8	14	0	134	142	1	34	1	30	23	6	8	1	136	128
0	12	0	323	- 545	8	19	0	54	- 52	2	1	1	208	168	6	9	1	86	- 80
0	14	0	491	- 480	8	20	0	150	157	2	4	1	272	240	6	10	1	128	- 108
0	16	0	507	492	8	22	0	70	69	2	6	1	153	155	6	11	1	65	72
0	20	0	75	78	8	24	0	49	46	2	7	1	187	169	6	12	1	60	- 69
0	22	0	79	75	8	28	0	46	- 41	2	8	1	339	- 294	6	13	1	97	103
0	24	0	163	173	8	29	0	35	29	2	9	1	108	- 109	6	14	1	31	- 36
0	26	0	154	166	8	30	0	43	38	2	10	1	129	124	6	15	1	39	51
0	28	0	38	- 38	10	1	0	74	85	2	11	1	139	- 121	6	17	1	29	28
0	30	0	67	- 64	10	2	0	69	- 84	2	12	1	29	22	6	20	1	31	- 25
0	32	0	73	- 53	10	3	0	49	64	2	14	1	302	- 297	6	26	1	30	- 21
2	1	0	194	206	10	4	0	63	- 83	2	15	1	90	- 84	6	28	1	39	- 34
2	2	0	35	- 26	10	5	0	120	- 144	2	16	1	25	20	6	29	1	30	- 20
2	5	0	212	- 232	10	7	0	207	- 247	2	17	1	35	- 40	7	1	1	209	- 183
2	6	0	147	157	10	8	0	209	247	2	18	1	61	- 74	7	2	1	22	- 27
2	7	0	583	551	10	10	0	191	229	2	19	1	57	76	7	4	1	36	42
2	9	0	176	- 170	10	11	0	159	152	2	20	1	33	12	7	7	1	38	- 31
2	10	0	567	545	10	12	0	38	35	2	21	1	48	48	7	8	1	171	166
2	11	0	173	- 196	10	14	0	98	102	2	22	1	93	- 99	7	9	1	78	94
2	12	0	472	491	10	15	0	99	96	2	23	1	152	158	7	10	1	144	- 133
2	13	0	226	240	10	16	0	105	102	2	24	1	141	- 153	7	11	1	142	134
2	14	0	461	438	10	17	0	70	72	2	26	1	56	71	7	12	1	73	- 66
2	15	0	158	150	10	19	0	89	99	3	1	1	272	- 231	7	13	1	119	121
2	16	0	114	- 126	10	21	0	72	73	3	3	1	322	334	7	14	1	54	- 47
2	17	0	78	61	10	22	1	92	- 89	3	4	1	321	311	7	15	1	53	40
2	18	0	340	- 355	10	23	1	100	- 119	3	5	1	398	434	7	16	1	32	- 31
2	20	0	60	- 64	10	26	0	41	51	3	6	1	311	322	7	17	1	74	- 81
2	21	0	62	- 68	12	1	0	77	- 87	3	7	1	160	- 183	7	18	1	50	- 61
2	22	0	85	- 84	12	2	0	77	106	3	8	1	210	196	7	19	1	44	- 51
2	23	0	89	115	12	3	0	65	- 57	3	9	1	133	- 110	7	20	1	83	- 81
2	24	0	70	- 74	12	5	0	172	195	3	10	1	33	- 30	7	22	1	45	55
2	25	0	112	114	12	6	0	56	- 57	3	11	1	71	- 67	7	24	1	93	102
2	27	0	44	- 43	12	7	0	139	154	3	12	1	69	- 70	8	1	1	75	- 69
2	28	0	87	90	12	8	0	64	- 68	3	13	1	33	- 26	8	2	1	108	96
2	30	0	67	76	12	10	0	62	- 63	3	14	1	212	- 199	8	3	1	187	171
4	1	0	297	312	12	11	0	62	- 60	3	15	1	76	83	8	4	1	58	47
4	2	0	235	246	12	13	0	38	- 51	3	16	1	274	- 261	8	5	1	90	- 87
4	3	0	55	55	12	15	0	54	79	3	17	1	179	- 174	8	6	1	127	- 101
4	5	0	29	34	12	18	0	41	48	3	20	1	83	- 73	8	7	1	41	- 45
4	6	0	59	- 69	12	19	0	59	- 65	3	21	1	142	140	8	8	1	173	- 166
4	7	0	40	- 48	12	22	0	43	59	3	24	1	75	80	8	9	1	53	- 56
4	8	0	45	- 51	12	23	0	48	56	3	28	1	69	81	8	10	1	93	86
4	9	0	166	181	14	1	0	74	84	3	31	1	36	46	8	11	1	56	- 60
4	10	0	322	- 327	14	2	0	74	- 91	3	32	1	35	- 42	8	13	1	29	- 33
4	11	0	574	600	14	3	0	44	48	4	1	1	67	63	8	14	1	122	- 124
4	12	0	220	- 219	14	5	0	66	- 71	4	2	1	123	118	8	15	1	60	- 66
4	13	0	78	- 70	14	7	0	53	- 55	4	3	1	453	- 404	8	16	1	35	- 36
4	14	0	58	66	14	8	0	53	- 50	4	4	1	129	- 138	8	18	1	36	- 47
4	15	0	163	- 169	14	10	0	31	29	4	5	1	95	87	8	20	1	51	60
4	16	0	37	47	14	11	0	36	40	4	6	1	268	222	8	21	1	59	66
4	18	0	134	139	14	12	0	60	59	4	7	1	116	98	8	24	1	70	- 74
4	19	0	58	57	14	18	0	78	- 56	4	8	1	320	- 295	9	3	1	100	105
4	20	0	52	54	14	19	0	40	34	4	9	1	268	256	9	4	1	51	- 51
4	21	0	145	151	14	20	0	31	- 25	4	10	1	264	- 238	9	5	1	38	- 30
4	22	0	54	- 49	16	12	0	57	- 52	4	11	1	304	270	9	6	1	316	- 300
4	23	0	55	- 62	16	14	0	51	- 41	4	12	1	114	112	9	7	1	36	- 37
4	25	0	73	- 86	16	16	0	34	38	4	13	1	116	- 111	9	8	1	51	- 49
4	28	0	70	- 62	0	8	1	60	- 65	4	15	1	142	146	9	9	1	90	- 82
6	1	0	89	98	0	10	1	376	- 388	4	16	1	160	166	9	10	1	91	107
6	2	0	301	- 290	0	12	1	58	- 52	4	17	1	217	210	9	11	1	124	- 135
6	3	0	122	- 138	0	14	1	86	87	4	20	1	59	- 62	9	12	1	84	98
6	4	0	108	- 136	0	16	1	227	232	4	22	1	57	49	9	14	1	85	76
6	5	0	64	- 55	0	18	1	86	- 91	4	23	1	44	- 53	9	16	1	31	- 35
6	6	0	29	22	0	19	1	33	29	4	24	1	38	- 46	9	17	1	31	- 30
6	7	0	385	412	0	20	1	188	- 184	4	26	1	31	- 20	9	18	1	94	66
6	10	0	402	456	0	22	1	67	- 69	4	27	1	59	64	9	19	1	51	56
6	11	0	59	- 75	0	24	1	119	- 114	5	3	1	134	- 112	9	20	1	51	67
6	12	0	43	- 49	0	26	1	183	- 155	5	5	1	303	- 180	9	22	1	43	- 47
6	13	0	128	129	0	28	1	76	- 86	5	7	1	119	120	9	24	1	28	- 33
6	14	0	78	- 68	1	1	1	67	- 53	5	8	1	196	- 192	10	3	1	57	- 55
6	16	0	70	72	1	2	1	157	- 130	5	9	1	81	92	10	5	1	58	- 65
6	17	0	65	53	1	5	1	38	44	5	12	1	122	129	10	6	1	85	88
6	18	0	88	- 102	1	6	1	54	- 57	5	13	1	126	- 135	10	7	1	232	224
6	21	0	98	- 105	1	8	1	26	27	5	14	1	114	114	10	9	1	127	122
6	22	0	78	- 87	1	7	1	260	249	5	15	1	103	112	10	10	1	137	- 146
6	24	0	45	- 37	1	9	1	90	- 90	5	17	1	127	134	10	12	1	43	- 44
6	26	0	53	55	1	11	1	152	159	5	18	1	128	132	10	13	1	36	- 34
6	27	0	58	- 48	1	12	1	152	133	5	19	1	48	58	10	14	1	36	- 27
8	1	0	105	107	1	13	1	162	- 164	5	20	1	49	62	10	17	1	85	113
8	2	0	144	166	1	14	1	443	419	5	21	1	36	- 38	10	20	1	72	- 69
8	3	0	128	157	1	15	1	127	- 116	5	24	1	61	- 76	10	21	1	42	- 50
8	4	0	353	376	1	16	1	198	194	5	25	1	51	59	11	2	1	42	- 46
8	5	0	271	276	1	17	1	133	181	5	26	1	43	- 36	11	3	1	58	- 64

Table 5. Continued.

H	K	L	FO	FC
11	4	1	128	124
11	5	1	59	- 53
11	6	1	114	105
11	7	1	43	31
11	8	1	66	63
11	9	1	145	146
11	10	1	50	55
11	12	1	75	- 90
11	13	1	75	- 76
11	14	1	64	- 63
11	16	1	36	- 29
11	18	1	99	- 87
11	22	1	43	36
11	23	1	36	- 37
12	1	1	66	- 65
12	3	1	140	154
12	4	1	99	- 104
12	5	1	114	116
12	6	1	31	- 33
12	8	1	45	- 30
12	9	1	45	- 37
12	10	1	45	- 52
12	13	1	79	77
12	16	1	35	25
12	18	1	61	51
12	19	1	28	33
12	21	1	60	59
13	1	1	45	39
13	2	1	89	- 75
13	4	1	61	- 62
13	5	1	129	125
13	6	1	53	- 53
13	7	1	50	- 52
13	8	1	44	- 37
13	9	1	112	- 107
13	14	1	56	52
13	16	1	51	49
13	21	1	44	39
14	1	1	89	82
14	2	1	35	29
14	3	1	35	- 44
14	4	1	43	51
14	6	1	30	- 31
14	7	1	30	30
14	9	1	48	46
14	11	1	33	34
14	13	1	27	- 31
15	2	1	69	71
15	4	1	33	32
15	9	1	49	50
15	15	1	38	- 36
16	4	1	30	36
17	1	1	41	32
17	2	1	41	- 41
3	0	2	31	- 29
4	0	2	188	195
5	0	2	228	226
6	0	2	502	- 527
7	0	2	101	- 103
9	0	2	181	167
10	0	2	145	- 137
11	0	2	84	73
12	0	2	79	75
13	0	2	76	- 74
15	0	2	87	66
16	0	2	44	31
17	0	2	47	- 33
0	2	2	172	- 174
0	4	2	176	- 166
0	6	2	163	- 170
0	8	2	230	- 229
0	10	2	533	- 573
0	12	2	61	- 63
0	14	2	189	- 188
0	16	2	78	- 80
0	18	2	251	240
0	22	2	78	69
0	26	2	92	- 87
0	30	2	44	- 35
0	32	2	41	- 37
1	4	2	65	69
1	5	2	156	- 164
1	6	2	175	191
1	7	2	235	251
1	8	2	201	- 207
1	9	2	125	128
1	10	2	184	187
1	11	2	25	- 28
1	12	2	286	279
1	13	2	57	54
1	14	2	253	271
1	15	2	69	- 65
1	16	2	112	- 109
1	18	2	217	- 204
1	22	2	39	- 46
1	23	2	139	130
1	26	2	79	- 64
1	28	2	71	- 57
1	30	2	83	74
2	1	2	110	115
2	3	2	379	- 404
2	4	2	426	- 469
2	5	2	389	- 398
2	6	2	19	16
2	7	2	123	118
2	8	2	145	148
2	9	2	222	- 226
2	10	2	200	218
2	11	2	37	- 41
2	12	2	78	79
2	13	2	63	56
2	14	2	62	- 56
2	15	2	118	- 121
2	16	2	62	66
2	17	2	55	43
2	18	2	110	- 111
2	20	2	130	- 120
2	24	2	51	- 53
2	25	2	46	- 36
2	27	2	49	- 47
2	32	2	45	41
3	1	2	223	229
3	2	2	60	- 72
3	3	2	347	358
3	4	2	31	- 39
3	5	2	167	- 181
3	6	2	160	- 162
3	7	2	276	- 295
3	8	2	59	- 58
3	9	2	129	135
3	11	2	280	281
3	12	2	261	- 251
3	14	2	80	- 79
3	15	2	170	- 175
3	16	2	49	50
3	17	2	64	- 59
3	18	2	35	39
3	19	2	36	25
3	20	2	104	91
3	23	2	78	- 74
3	24	2	46	- 33
3	25	2	56	- 52
3	27	2	64	57
4	1	2	109	102
4	2	2	161	171
4	3	2	106	114
4	4	2	99	97
4	6	2	81	- 83
4	8	2	280	- 267
4	9	2	90	- 94
4	10	2	209	- 205
4	11	2	93	- 86
4	12	2	130	- 126
4	13	2	47	- 44
4	14	2	89	- 94
4	15	2	158	- 165
4	18	2	97	93
4	20	2	159	163
4	21	2	72	- 64
4	22	2	98	95
4	23	2	80	78
4	28	2	45	- 46
4	31	2	46	- 45
5	1	2	60	- 57
5	2	2	88	- 94
5	3	2	326	- 353
5	4	2	115	- 122
5	5	2	144	154
5	6	2	200	199
5	7	2	299	317
5	8	2	115	114
5	9	2	238	- 242
5	11	2	76	- 91
5	12	2	74	- 67
5	13	2	49	- 38
5	14	2	132	- 118
5	15	2	86	80
5	16	2	46	41
5	17	2	90	74
5	18	2	105	93
5	19	2	226	- 194
5	20	2	55	- 52
5	22	2	69	- 53
5	23	2	59	56
6	1	2	240	- 246
6	2	2	209	- 230
6	3	2	83	- 77
6	4	2	99	- 102
6	5	2	86	- 86
6	6	2	77	76
6	7	2	158	- 151
6	8	2	364	354
6	10	2	92	82
6	11	2	130	- 129
6	12	2	95	97
6	13	2	57	59
6	14	2	49	42
6	15	2	88	86
6	16	2	62	- 59
6	17	2	53	- 50
6	20	2	113	- 112
6	22	2	94	- 72
6	28	2	38	34
6	30	2	40	42
7	1	2	100	95
7	2	2	115	111
7	3	2	132	137
7	4	2	320	310
7	5	2	126	- 129
7	7	2	52	- 55
7	8	2	179	- 176
7	9	2	52	50
7	10	2	53	- 48
7	12	2	84	83
7	14	2	160	148
7	15	2	117	- 99
7	16	2	64	- 57
7	18	2	97	- 90
7	19	2	91	89
7	20	2	89	89
7	22	2	79	71
8	1	2	58	50
8	2	2	171	173
8	5	2	93	- 92
8	6	2	136	- 127
8	8	2	103	- 95
8	10	2	248	- 228
8	12	2	147	- 135
8	13	2	43	- 49
8	14	2	77	- 65
8	15	2	129	- 124
8	16	2	78	- 64
8	18	2	54	48
8	19	2	46	41
8	20	2	71	59
8	28	2	23	- 25
9	4	2	223	- 204
9	5	2	49	- 38
9	6	2	81	- 71
9	7	2	169	- 157
9	8	2	156	139
9	9	2	65	- 57
9	10	2	171	152
9	11	2	114	110
9	15	2	45	46
9	16	2	71	69
9	17	2	71	60
9	18	2	46	42
9	20	2	55	- 47
9	22	2	82	- 73
9	25	2	37	- 36
9	26	2	30	27
10	2	2	76	- 57
10	3	2	78	- 64
10	4	2	77	- 64
10	5	2	42	- 34
10	6	2	88	- 81
10	8	2	89	80
10	9	2	66	- 57
10	10	2	50	41
10	16	2	92	- 85
10	18	2	86	- 74
10	19	2	54	- 51
10	22	2	63	- 58
11	1	2	38	45
11	2	2	38	- 33
11	3	2	95	- 87
11	4	2	69	55
11	5	2	65	53
11	7	2	250	212
11	8	2	144	- 132
11	11	2	55	- 46
11	19	2	96	- 71
11	25	2	26	30
12	1	2	93	- 73
12	3	2	98	83
12	5	2	69	55
12	6	2	46	38
12	7	2	76	- 79
12	8	2	86	- 72
12	9	2	97	80
12	10	2	69	- 52
12	12	2	58	- 48
12	13	2	78	- 71
12	14	2	54	- 52
12	17	2	51	- 51
13	5	2	58	- 54
13	7	2	58	- 58
13	11	2	93	83
13	12	2	53	34
13	15	2	67	- 55
13	16	2	48	- 27
13	18	2	42	- 36
14	3	2	58	- 48
14	5	2	57	- 48
14	12	2	39	31
14	13	2	38	36
15	2	2	46	30
15	4	2	62	- 48
15	8	2	65	50
15	12	2	34	- 28
15	19	2	30	- 20
16	2	2	42	36
16	3	2	25	21
16	5	2	41	31
16	6	2	29	- 21
16	7	2	33	25
16	13	2	26	- 19
17	3	2	24	- 23
17	4	2	55	42
17	6	2	35	21
0	2	3	124	- 131
0	4	3	185	- 185
0	6	3	130	129
0	8	3	100	- 96
0	10	3	140	- 121
0	12	3	81	81
0	14	3	76	72
0	16	3	258	245
0	18	3	77	75
0	20	3	97	- 86
0	24	3	69	57
0	26	3	37	29
1	1	3	182	198
1	2	3	46	- 52
1	3	3	37	35
1	4	3	281	- 284
1	5	3	184	178
1	6	3	266	- 259
1	7	3	208	- 185
1	8	3	97	- 106
1	9	3	156	- 140
1	10	3	102	91
1	11	3	83	75
1	12	3	181	171
1	13	3	74	76
1	15	3	84	82
1	18	3	114	110
1	20	3	101	95
1	23	3	47	43
1	24	3	54	- 42
1	26	3	52	- 47
1	29	3	40	36
1	31	3	27	- 31
2	1	3	64	- 68
2	2	3	287	309
2	3	3	71	67
2	4	3	66	- 58
2	5	3	145	140
2	6	3	120	105
2	7	3	111	- 107
2	8	3	46	43
2	9	3	198	- 198
2	12	3	72	82
2	14	3	101	- 102
2	15	3	32	- 38
2	16	3	111	- 115
2	17	3	136	- 126
2	19	3	87	- 89
2	20	3	74	69
2	22	3	78	78
2	26	3	66	62
2	28	3	63	61
3	1	3	65	65
3	2	3	216	217
3	3	3	231	- 225
3	4	3	88	- 86
3	5	3	462	- 452
3	6	3	287	298
3	8	3	115	110
3	9	3	240	234
3	10	3	26	- 35
3	11	3	66	74
3	13	3	65	55
3	14	3	206	- 186
3	16	3	54	- 51
3	19	3	58	- 60
3	21	3	125	- 132
3	22	3	61	70
3	24	3	66	71
3	26	3	58	50
4	1	3	332	330
4	2	3	380	- 366
4	3	3	63	- 53

Table 5. Continued.

H	K	L	FO	FC
4	4	3	32	- 27
4	5	3	289	- 287
4	6	3	394	- 396
4	7	3	83	- 94
4	8	3	123	- 144
4	9	3	95	100
4	10	3	134	144
4	11	3	115	- 109
4	13	3	134	- 146
4	14	3	94	97
4	16	3	122	111
4	18	3	80	86
4	20	3	68	62
4	21	3	84	- 75
4	25	3	45	44
5	1	3	200	- 197
5	2	3	183	- 179
5	3	3	134	135
5	4	3	190	- 199
5	5	3	47	- 47
5	7	3	180	- 174
5	8	3	156	- 154
5	9	3	216	- 220
5	10	3	97	- 107
5	11	3	94	- 108
5	12	3	89	76
5	13	3	93	98
5	14	3	158	155
5	16	3	139	151
5	17	3	86	- 88
5	20	3	61	- 53
5	21	3	51	- 44
5	24	3	44	- 38
5	27	3	43	- 56
6	1	3	117	- 102
6	2	3	53	49
6	3	3	54	64
6	4	3	134	141
6	5	3	116	116
6	6	3	257	279
6	8	3	203	218
6	9	3	120	- 116
6	10	3	57	- 66
6	11	3	76	96
6	13	3	176	162
6	15	3	44	- 50
6	16	3	58	- 57
6	17	3	67	- 63
6	18	3	85	- 82
6	19	3	47	- 45
6	22	3	47	- 57
6	24	3	84	77
6	26	3	41	43
7	2	3	249	273
7	4	3	151	172
7	5	3	67	- 60
7	6	3	38	50
7	7	3	83	96
7	8	3	62	61
7	10	3	81	81
7	11	3	103	- 107
7	12	3	43	- 50
7	14	3	170	- 196
7	16	3	176	- 175
7	21	3	60	- 64
8	1	3	51	49
8	2	3	118	135
8	3	3	49	58
8	4	3	127	- 147
8	6	3	53	- 55
8	7	3	41	- 53
8	8	3	59	- 65
8	10	3	113	116
8	11	3	115	- 117
8	12	3	169	196
8	13	3	94	- 101
8	14	3	65	- 68
8	15	3	46	51
8	18	3	64	69
8	24	3	47	- 49
9	1	3	59	64
9	2	3	101	- 105
9	3	3	76	77
9	4	3	148	- 170
9	5	3	72	- 72
9	8	3	80	- 82
9	9	3	78	80
9	10	3	94	- 93
9	14	3	61	61
9	16	3	126	134
9	24	3	38	- 32
10	2	3	88	- 103
10	3	3	88	- 96
10	4	3	88	103
10	6	3	64	73
10	8	3	95	100
10	11	3	38	29
10	12	3	67	- 70
10	13	3	58	- 57
10	14	3	60	43
10	15	3	46	- 62
10	21	3	33	- 34
11	1	3	53	- 62
11	2	3	46	46
11	3	3	46	50
11	4	3	123	123
11	12	3	46	- 46
11	13	3	89	95
12	1	3	78	- 85
12	7	3	61	- 65
12	9	3	81	- 85
12	11	3	37	- 34
12	14	3	44	44
12	22	3	24	- 24
13	1	3	45	44
13	2	3	183	- 179
13	5	3	45	- 55
13	6	3	45	- 42
13	9	3	26	- 28
13	10	3	26	37
13	11	3	43	- 31
13	13	3	34	- 31
14	1	3	56	- 40
14	2	3	53	60
14	3	3	50	- 49
14	9	3	46	45
14	12	3	36	34
14	14	3	33	- 33
15	2	3	36	- 23
15	3	3	32	- 21
15	6	3	56	60
15	9	3	23	23
15	11	3	27	- 30
15	13	3	26	- 24
16	2	3	42	- 40
16	6	3	28	17
16	7	3	25	- 25
1	0	4	178	- 207
2	0	4	65	60
3	0	4	178	183
4	0	4	183	179
5	0	4	192	- 188
6	0	4	163	- 159
7	0	4	22	27
8	0	4	179	166
9	0	4	140	- 134
10	0	4	184	- 169
11	0	4	42	38
12	0	4	46	40
0	2	4	143	156
0	4	4	301	309
0	6	4	172	185
0	8	4	169	- 166
0	10	4	169	- 175
0	12	4	109	109
0	16	4	45	49
0	22	4	156	161
0	24	4	49	- 54
0	26	4	77	- 80
0	30	4	26	- 32
1	1	4	73	93
1	2	4	71	- 66
1	3	4	28	30
1	4	4	99	94
1	5	4	28	- 25
1	6	4	145	133
1	7	4	66	- 69
1	8	4	100	97
1	9	4	137	- 137
1	10	4	68	63
1	11	4	43	- 43
1	12	4	110	105
1	14	4	60	58
1	15	4	47	48
1	17	4	36	41
1	21	4	31	- 30
1	22	4	39	- 44
1	23	4	31	- 40
1	30	4	21	23
2	1	4	137	137
2	2	4	37	21
2	3	4	267	276
2	4	4	59	- 67
2	5	4	30	30
2	6	4	128	120
2	7	4	54	- 61
2	8	4	278	285
2	9	4	88	87
2	10	4	124	130
2	11	4	99	99
2	12	4	44	39
2	13	4	63	57
2	14	4	64	- 54
2	15	4	99	- 86
2	16	4	29	- 30
2	18	4	43	46
2	19	4	65	65
2	20	4	65	- 72
2	21	4	60	- 55
2	22	4	75	- 76
2	23	4	91	- 40
2	28	4	31	34
2	29	4	54	50
3	2	4	253	247
3	3	4	78	78
3	4	4	81	86
3	5	4	166	169
3	7	4	106	105
3	8	4	60	54
3	9	4	46	46
3	10	4	96	- 98
3	11	4	35	- 29
3	12	4	134	- 122
3	13	4	86	- 86
3	17	4	30	- 31
3	18	4	56	56
3	20	4	70	50
3	21	4	57	61
3	22	4	61	62
3	24	4	50	52
4	1	4	138	- 132
4	2	4	278	269
4	3	4	70	- 70
4	4	4	103	108
4	5	4	146	145
4	6	4	82	- 78
4	7	4	105	102
4	8	4	45	44
4	10	4	104	- 111
4	11	4	110	- 102
4	12	4	102	- 103
4	13	4	48	52
4	16	4	146	144
4	17	4	31	28
4	18	4	44	47
4	19	4	31	- 37
4	20	4	39	32
4	21	4	44	- 46
4	22	4	31	35
4	23	4	37	36
4	24	4	30	25
4	27	4	31	- 27
5	2	4	136	- 134
5	3	4	27	28
5	4	4	73	- 74
5	6	4	61	51
5	7	4	96	- 89
5	8	4	56	48
5	10	4	105	102
5	12	4	224	211
5	13	4	29	31
5	15	4	92	97
5	16	4	81	- 73
5	17	4	84	80
5	18	4	57	- 51
5	19	4	45	43
5	20	4	83	- 83
5	23	4	30	- 30
5	24	4	29	- 30
6	1	4	205	210
6	2	4	44	- 48
6	3	4	34	37
6	4	4	83	83
6	5	4	88	- 81
6	6	4	55	55
6	7	4	26	- 26
6	8	4	23	- 23
6	9	4	78	- 78
6	10	4	34	37
6	11	4	198	189
6	12	4	203	200
6	13	4	30	25
6	14	4	113	119
6	15	4	80	- 75
6	16	4	62	- 64
6	17	4	96	96
6	18	4	66	- 61
6	25	4	26	- 41
7	1	4	67	72
7	2	4	73	73
7	3	4	79	78
7	5	4	45	47
7	6	4	66	- 59
7	7	4	61	52
7	8	4	59	- 65
7	9	4	66	- 55
7	10	4	181	- 168
7	11	4	59	- 55
7	12	4	177	- 177
7	13	4	31	32
7	14	4	81	- 79
7	20	4	37	35
7	22	4	29	33
8	2	4	107	99
8	3	4	52	54
8	4	4	98	- 108
8	5	4	47	45
8	6	4	94	- 107
8	7	4	54	53
8	8	4	118	104
8	9	4	71	66
8	10	4	30	29
8	11	4	31	- 26
8	12	4	78	- 78
8	13	4	33	39
8	17	4	38	- 41
8	18	4	84	89
8	22	4	24	- 32
8	26	4	21	16
9	1	4	69	- 78
9	2	4	51	- 57
9	4	4	40	- 45
9	7	4	64	- 59
9	8	4	74	65
9	9	4	61	54
9	10	4	31	20
9	13	4	63	- 57
9	20	4	28	- 29
9	22	4	25	- 28
9	24	4	22	- 25
10	1	4	137	- 136
10	4	4	38	- 33
10	6	4	72	66
10	8	4	28	32
10	11	4	43	- 38
10	12	4	45	34
10	13	4	84	87
10	14	4	31	- 27
10	15	4	46	41
10	16	4	33	- 34
11	2	4	31	41
11	3	4	31	29
11	5	4	39	33
11	7	4	31	27
11	8	4	31	- 26
11	11	4	31	- 38
11	12	4	30	37
11	14	4	29	- 24
11	17	4	33	- 35
11	22	4	42	42
12	1	4	73	66
12	2	4	31	25
12	3	4	41	42
12	4	4	31	25
12	5	4	31	- 32
12	15	4	44	- 40
12	18	4	23	26
12	19	4	42	32
12	20	4	42	31
12	21	4	40	38
13	5	4	47	- 36
13	7	4	35	- 33
13	8	4	34	42
13	13	4	35	36
13	16	4	21	19
13	17	4	36	34
14	1	4	33	- 33
14	2	4	33	- 30
14	3	4	38	- 27
14	4	4	53	- 44
14	8	4	61	44
14	10	4	54	45
14	15	4	35	35
15	5	4	44	37
15	7	4	39	34
15	9	4	24	22
15	10	4	19	- 21
15	11	4	22	- 22
16	4	4	35	29
0	4	5	125	- 124
0	6	5	261	- 258
0	8	5	39	- 41
0	10	5	41	38
0	12	5	107	101
0	14	5	65	60
0	16	5	46	- 54
0	18	5	93	91
0	22	5	61	- 56
0	26	5	75	- 71
0	28	5	32	- 16
1	1	5	9	- 12
1	2	5	52	57
1	3	5	13	- 25

Table 5. Continued.

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	4	5	68	- 70	3	12	5	22	- 21	6	4	5	122	107	10	11	5	72	62
1	5	5	37	44	3	13	5	45	- 55	6	7	5	48	45	10	13	5	53	48
1	6	5	280	- 258	3	15	5	43	- 52	6	9	5	89	88	10	14	5	61	- 57
1	7	5	16	- 19	3	16	5	49	- 52	6	11	5	27	41	10	16	5	21	- 28
1	8	5	171	- 162	3	17	5	89	105	6	14	5	78	- 76	10	17	5	23	- 26
1	9	5	56	- 53	3	18	5	39	- 39	6	15	5	28	25	10	18	5	22	- 23
1	10	5	80	87	3	19	5	57	67	6	16	5	112	- 123	10	19	5	21	- 22
1	12	5	119	120	3	22	5	27	35	6	24	5	22	20	11	1	5	62	- 61
1	15	5	32	- 39	4	1	5	43	- 41	7	2	5	97	90	11	4	5	39	32
1	16	5	27	25	4	2	5	90	- 86	7	4	5	69	70	11	5	5	38	39
1	17	5	34	- 38	4	3	5	20	26	7	6	5	37	- 39	11	8	5	33	25
1	18	5	68	73	4	4	5	125	- 110	7	7	5	45	47	11	9	5	39	- 42
1	19	5	62	- 65	4	5	5	118	124	7	9	5	27	35	11	11	5	25	22
1	21	5	24	22	4	5	6	69	- 74	7	12	5	34	39	11	13	5	34	40
1	24	5	34	- 43	4	7	5	55	- 53	7	15	5	44	- 45	11	14	5	51	- 47
2	1	5	69	- 68	4	8	5	67	- 61	7	16	5	49	- 51	11	16	5	47	- 45
2	2	5	59	- 64	4	9	5	114	- 115	7	19	5	37	36	11	17	5	32	- 33
2	3	5	56	- 46	4	11	5	22	18	7	20	5	31	28	12	1	5	87	75
2	4	5	207	185	4	12	5	26	26	8	1	5	27	30	12	4	5	41	- 42
2	5	5	118	- 109	4	13	5	32	34	8	2	5	193	- 177	12	6	5	36	- 36
2	6	5	125	125	4	14	5	30	41	8	3	5	48	48	12	8	5	25	- 24
2	7	5	50	50	4	16	5	58	62	8	4	5	27	- 19	12	13	5	40	- 41
2	8	5	161	153	4	21	5	47	59	8	5	5	24	- 27	13	1	5	42	39
2	9	5	154	157	4	22	5	26	- 28	8	6	5	104	- 98	13	2	5	34	- 22
2	10	5	20	29	4	23	5	25	27	8	8	5	28	- 43	13	5	5	53	- 49
2	11	5	49	- 44	4	24	5	45	- 48	8	10	5	28	- 43	13	6	5	42	- 34
2	12	5	123	- 122	4	25	5	28	- 35	8	12	5	68	- 69	13	9	5	53	48
2	15	5	50	44	4	26	5	35	- 38	8	14	5	114	112	14	2	5	25	- 29
2	16	5	109	- 103	5	1	5	68	- 72	8	15	5	34	37	14	6	5	19	23
2	18	5	92	- 89	5	2	5	77	- 69	8	16	5	48	59	0	6	6	87	- 86
2	19	5	39	44	5	3	5	78	76	8	17	5	27	19	0	12	6	44	- 32
2	20	5	24	- 33	5	4	5	51	- 53	8	19	5	25	36	0	14	6	53	53
2	21	5	39	- 46	5	5	5	116	110	8	22	5	21	- 18	0	16	6	43	27
2	22	5	44	- 48	5	7	5	54	58	9	2	5	105	- 92	0	20	6	33	36
2	24	5	31	35	5	8	5	82	79	9	4	5	34	- 28	0	4	7	133	- 140
2	25	5	24	26	5	9	5	25	34	9	5	5	28	- 35	0	6	7	117	- 129
3	1	5	42	45	5	10	5	73	74	9	11	5	85	- 84	0	8	7	72	- 79
3	2	5	17	- 16	5	11	5	26	43	9	13	5	71	- 62	0	12	7	50	54
3	3	5	36	31	5	12	5	23	49	9	14	5	53	54	0	14	7	39	37
3	4	5	76	- 71	5	13	5	55	62	9	16	5	65	63	0	16	7	31	29
3	6	5	139	137	5	15	5	44	47	9	20	5	22	- 20	0	18	7	47	52
3	7	5	144	136	5	20	5	55	- 33	10	1	5	51	- 43	0	20	7	46	55
3	8	5	84	85	5	21	5	37	53	10	2	5	44	46	0	10	8	33	37
3	9	5	46	48	5	25	5	20	- 19	10	3	5	24	- 20	0	12	8	31	- 30
3	10	5	90	- 100	6	2	5	170	155	10	4	5	28	35	0	14	8	28	- 31
3	11	5	52	- 47	6	3	5	70	- 66	10	5	5	53	58					

RESULTS

The final atomic coordinates and temperature parameters are listed in Tables 1 and 2, respectively. Bond lengths and bond angles as calculated from the coordinates in Table 1, are listed in Tables 3 and 4.

The equations for some least squares planes, and deviations from these planes for certain atoms are given below. X, Y, and Z are in Å units and the notation of the planes are the same as on Figs. 1 and 2.

Ring A. (Double weight on sulphur)

$$-0.57661\,X - 0.46735\,Y + 0.67016\,Z = -2.44759$$

Deviations in Å units: S_1 (−0.006), S_2 (0.006), C_1 (0.012), C_2 (−0.002), C_3 (−0.009), C_4 (0.009), C_5 (0.047), O (0.022), C_6 (0.037), C_9 (0.103), C_{12} (0.016) and C_{15} (−0.094).

Ring B

$$-0.33129\,X - 0.25056\,Y + 0.90965\,Z = -0.65542$$

Deviations in Å units: C_6 (−0.006), C_7 (0.008), C_8 (−0.004), C_9 (−0.001), C_{10} (0.002) and C_{11} (0.001).

The angle between the normal to A and the normal to B is 23.4°.

Ring D

$$-0.14864\,X + 0.96246\,Y - 0.22712\,Z = 3.09404$$

Deviations in Å units: C_{12} (−0.002), C_{13} (0.008), C_{14} (−0.011), C_{15} (0.008), C_{16} (−0.001), C_{17} (−0.001) and C_4 (0.103).

The angle between the normal to D and the normal to A is 119.6°.

The bond $C_{12}-C_4$ forms an angle of 3.7° with the least squares plane of ring *D*.

*Ring A*1 (single weight on sulphur)

$0.57738\,X - 0.46520\,Y + 0.67098\,Z = -4.78116$

*Ring B*2

$-0.33129\,X + 0.25056\,Y + 0.90965\,Z = 6.09177$

The angle between the normal to *A*1 and the normal to *B*2 is 72.4°.

*Ring B*3

$-0.33129\,X + 0.25056\,Y + 0.90965\,Z = 2.67190$

The distance between the parallel planes of *B*2 and *B*3 is thus 3.42 Å.

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