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The Crystal and Molecular Structure of β-Thianthrene Dioxide, C_6H_4–$(SO)_2$–C_6H_4

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The crystal structure of β-thianthrene dioxide was determined by X-ray diffraction methods. Three-dimensional data collected visually from Weissenberg photographs were used in the final least-squares refinement by taking account of a different anisotropic temperature factor for each atom but entirely disregarding H atoms. According to the final results, with the reliability index of 10·7% for observed reflexions, the molecule is folded about the line joining the two heterocyclic sulphur atoms. The best planes for two benzene rings were found to make an angle of about 133°. The two S atoms lie slightly outside of this dihedral angle. The S–C and S–O bond lengths were 1·72–1·87 and 1·47–1·48 Å respectively. The two bond angles C–S–C were found to be 96–97°. It was definitely confirmed that the β isomer of thianthrene dioxide has the *trans* form regarding the position of the two oxygen atoms.

Introduction

Two isomers of thianthrene dioxide, C_6H_4–$(SO)_2$–C_6H_4 (Fig. 1), are known. Because of its low dipole moment the α isomer (m.p. 284°C) was considered by Bergmann & Tschudnowsky (1932) to be the *trans* isomer. Baw, Bennett & Dearns (1934) reached the same conclusion because they found the β form (m.p. 249°C) to be three times as soluble as the α form in glacial acetic acid. Taylor (1935) considered three possible molecular models for thianthrene dioxide (Fig. 2), which may be called the *anti-cis*, *syn-cis* and *trans* forms. His estimates of the dipole moments are as described in Fig. 2. He predicted that the α isomer, which has a dipole moment only slightly greater than that of thianthrene (1·4 to 1·55D according to solvent), has the *anti-cis* form, and the β isomer the *trans* form. As already reported (Hosoya & Wood, 1957; Hosoya, 1958*a*, *c*), preliminary X-ray analyses confirmed this prediction. The present author also reported on a preliminary X-ray analysis on thianthrene tetraoxide (Hosoya, 1958*b*, *c*). As for thianthrene, the detailed analyses have already been published (Lynton & Cox, 1956; Rowe & Post, 1958). Structural features of molecules of these four compounds have already been compared and discussed from a general point of view by use of the available data (Hosoya, 1958*c*, 1963). In the present article, a more detailed analysis based on three-dimensional data is described for β-thianthrene dioxide.

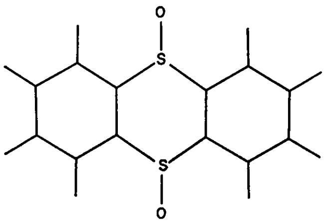

Fig. 1. Structural formula of β-thianthrene dioxide.

Experimental

Crystal data

$C_{12}H_8O_2S_2$: m.p. 249°C.

Monoclinic, $a=11·5\pm0·05$, $b=14·1\pm0·06$, $c=6·5\pm0·03$ Å; $\beta=92\pm0·5°$, $Z=4$.

Absent reflexions: $h0l$ when $h+l$ is odd; $0k0$ when k is odd. Space group $P2_1/n$.

Density: $d_{\text{calc}}=1·59$ g.cm^{-3}; $d_{\text{obs}}=1·56$ g.cm^{-3}.

Refractive indices: $\alpha=1·61(\|\mathbf{b})$, $\beta=1·77(\text{approx.}\|\mathbf{c})$, $\gamma=1·88(\text{approx.}\|\mathbf{a})$.

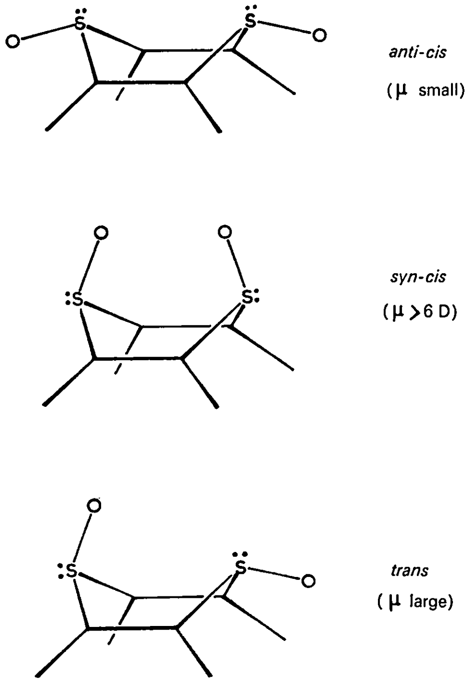

Fig. 2. Three possible molecular models of thianthrene dioxide.

Crystal habit

The crystal has the form of a prism, the cross-section being a parallelogram. The axis of this prism is found to be the *c* axis. The crystal is rather hard, has no layer or fibrous texture and does not show any prominent cleavage.

Intensity data

A spherical crystal, about 0·45 mm in diameter, was used for collecting the three-dimensional data. The linear absorption coefficient is 44·5 cm^{-1}, and the sphericity was of the order of ± 10%. The absorption correction was made graphically for the value of $\mu R = 1{\cdot}0$.

Solution of the structure

As the *c* edge is shortest, the (001) projection was chosen as the first one. The usual Patterson map did not show peaks clear enough to locate sulphur–sulphur peaks. The sharpened Patterson map, however, gave a correct clue to the unravelling of the structure. At this stage, the values of anisotropic refractive indices helped to solve the structure, because these data suggested that the molecule is more or less parallel to the (010) plane with its S–S line roughly along the *c* axis. The first Fourier map obtained with signs determined only by the sulphur contribution showed the outline of the molecule. Then the usual refinement was performed by repeating the F_c calculation and the Fourier synthesis alternately, by using a wire model, and lastly by a difference synthesis. At a fairly early stage, the positions of two oxygen atoms could be definitely determined corresponding to one of two possible ways to place the molecule. Several cycles of refinement with a fixed over-all temperature factor were carried out on an Elliott 402 computer, and the reliability index of the observed *hk*0 reflexions decreased to about 16%.

The (100) projection was chosen as the second one. The usual Patterson map, though it did not show clear peaks, could give information of the *z* parameters of sulphur atoms, since their *y* parameters were already known. Again by projecting the wire model on the map, all atoms except hydrogen atoms were located more or less accurately in spite of heavy overlaps. Then several cycles of similar refinement as above were carried out for this projection and the *R* index decreased to 22% for the observed reflexions.

Three-dimensional data were collected from the rotation photographs around the *b* axis. The values of

Table 1(*a*). *Final fractional atomic coordinates with standard deviations*

	x/a	$\sigma(x) \times 10^5$	y/b	$\sigma(y) \times 10^5$	z/c	$\sigma(z) \times 10^5$
S(1)	0·12590	27	0·26122	23	−0·10431	41
S(2)	0·13410	26	0·17114	23	0·35789	41
O(1)	0·12038	77	0·34309	60	0·03795	129
O(2)	0·14114	74	0·09709	65	0·51696	116
C(1)	0·34143	114	0·18105	102	−0·13882	191
C(2)	0·43967	127	0·13303	114	−0·07300	232
C(3)	0·44075	131	0·09227	108	0·13166	228
C(4)	0·34428	124	0·10202	96	0·26208	211
C(5)	−0·06734	105	0·08275	93	0·23857	194
C(6)	−0·16128	119	0·06507	101	0·09681	218
C(7)	−0·16580	117	0·10167	102	−0·09593	203
C(8)	−0·07474	98	0·16141	95	−0·16409	177
C(9)	0·01709	98	0·18045	88	−0·02651	170
C(10)	0·01871	100	0·13970	88	0·17493	164
C(11)	0·24925	98	0·15175	92	0·18714	177
C(12)	0·24911	101	0·19275	95	−0·01389	175

Table 1(*b*). *Anisotropic temperature factors* (Å^2) *with their standard deviations*

	$B_{11} \times 10^5$	$\sigma(B_{11}) \times 10^5$	$B_{22} \times 10^5$	$\sigma(B_{22}) \times 10^5$	$B_{33} \times 10^5$	$\sigma(B_{33}) \times 10^5$	$B_{23} \times 10^5$	$\sigma(B_{23}) \times 10^5$	$B_{31} \times 10^5$	$\sigma(B_{31}) \times 10^5$	$B_{12} \times 10^5$	$\sigma(B_{12}) \times 10^5$
S(1)	701	24	498	21	1612	64	123	29	25	31	−28	18
S(2)	705	23	573	20	1548	58	27	29	46	28	−35	19
O(1)	1010	85	449	56	2666	239	−18	91	−52	114	103	56
O(2)	891	77	735	63	2079	201	445	93	−143	99	−108	58
C(1)	700	112	596	95	2147	315	−51	143	88	154	−128	86
C(2)	725	132	679	109	3121	433	−283	173	36	191	−186	95
C(3)	947	141	520	99	3106	415	−292	167	−123	194	42	95
C(4)	888	129	348	84	2932	384	−379	140	−90	178	85	83
C(5)	676	98	491	86	2824	348	−104	138	212	149	−66	72
C(6)	816	121	600	96	3294	413	204	158	153	181	48	84
C(7)	832	121	607	93	2936	369	17	150	−201	165	118	86
C(8)	622	92	617	89	2187	295	−104	132	−149	135	−34	74
C(9)	619	93	500	79	1955	287	−19	121	−70	132	125	71
C(10)	610	95	524	82	1806	267	85	116	104	128	84	69
C(11)	499	90	436	81	2088	297	−20	122	−76	138	55	68
C(12)	604	95	518	89	1819	284	−11	123	78	135	−42	73

Table 2. *Observed and calculated structure factors*

H	K	L	F_o	F_c
2	0	0	10.37	8.18
4	0	0	102.09	-108.78
6	0	0	19.35	18.37
8	0	0	51.39	47.95
10	0	0	36.52	-33.92
14	0	0	5.97	6.43
1	1	0	41.10	45.18
2	1	0	61.95	-67.39
3	1	0	24.11	-22.65
4	1	0	10.29	11.59
5	1	0	5.71	8.34
6	1	0	72.52	69.19
7	1	0	14.41	19.40
8	1	0	7.82	-8.29
10	1	0	56.05	-48.94
14	1	0	8.19	9.67
0	2	0	99.45	-112.12
1	2	0	65.55	-68.62
2	2	0	6.59	6.58
4	2	0	34.49	36.53
8	2	0	43.99	-43.93
9	2	0	35.45	-36.81
10	2	0	4.56	3.67
12	2	0	8.78	11.07
1	3	0	27.29	-32.37
2	3	0	84.49	94.22
3	3	0	23.75	-20.26
4	3	0	11.53	13.04
5	3	0	10.01	-9.03
6	3	0	10.91	-8.52
7	3	0	17.76	-16.27
8	3	0	6.59	6.60
9	3	0	8.70	-8.60
12	3	0	10.01	-6.35
0	4	0	114.40	-113.50
1	4	0	47.17	51.46
2	4	0	20.05	-18.22
3	4	0	23.83	-21.73
4	4	0	3.32	-1.06
7	4	0	6.67	6.27
8	4	0	10.91	9.27
9	4	0	21.98	20.66
10	4	0	15.47	14.07
11	4	0	7.82	-7.29
12	4	0	10.91	-10.47
1	5	0	5.53	1.50
2	5	0	7.72	7.20
3	5	0	33.61	31.14
4	5	0	6.94	-7.79
7	5	0	7.82	-6.10
8	5	0	13.80	11.30
10	5	0	6.59	5.82
11	5	0	5.09	-4.17
14	5	0	2.80	3.78
0	6	0	11.43	11.62
1	6	0	7.46	10.32
3	6	0	20.59	18.77
4	6	0	26.22	22.96
6	6	0	6.67	-8.57
8	6	0	13.72	16.14
1	7	0	3.50	4.50
2	7	0	8.78	-10.37
3	7	0	5.13	6.18
4	7	0	4.12	-5.83
6	7	0	9.05	-8.52
7	7	0	8.44	8.83
8	7	0	7.46	-8.40
9	7	0	6.67	9.16
0	8	0	10.11	-8.47
1	8	0	11.35	-13.69
2	8	0	8.62	8.67
3	8	0	2.98	0.98
4	8	0	7.38	-6.66
5	8	0	5.71	5.70
6	8	0	5.23	-2.98
7	8	0	4.99	5.20
9	8	0	16.25	-13.03
10	8	0	6.05	4.31
12	8	0	6.77	-6.55
1	9	0	26.22	-28.67
2	9	0	27.28	-27.47
3	9	0	9.39	9.72
5	9	0	13.64	9.14
6	9	0	9.75	8.32
7	9	0	12.12	-11.71
8	9	0	4.99	-4.14
11	9	0	10.37	9.22
0	10	0	15.13	-13.48
1	10	0	20.98	20.68
2	10	0	5.21	-4.35
3	10	0	3.42	5.85
4	10	0	11.78	11.74
5	10	0	21.98	-22.90
6	10	0	5.35	6.16
7	10	0	11.60	-10.05
8	10	0	14.85	-14.43
9	10	0	17.50	17.42
11	10	0	5.21	4.94
12	10	0	5.79	5.47
1	11	0	19.71	19.92
2	11	0	22.26	24.85
3	11	0	14.85	-15.19
4	11	0	5.89	-6.60
5	11	0	16.52	-15.38
6	11	0	19.71	-19.77
7	11	0	9.75	10.08
8	11	0	5.61	6.31
9	11	0	5.97	6.34
10	11	0	10.45	11.88
11	11	0	6.33	-6.78
0	12	0	36.70	39.90
1	12	0	21.98	-22.61
3	12	0	16.82	-16.86
4	12	0	25.86	-26.28
5	12	0	16.62	17.69
7	12	0	7.02	4.63
8	12	0	11.68	10.56
9	12	0	9.85	-9.55
10	12	0	4.38	-4.88
2	13	0	15.83	-14.04
3	13	0	6.59	5.31
5	13	0	6.41	6.97
6	13	0	16.19	15.65
7	13	0	6.59	-5.85
9	13	0	8.44	-8.48
10	13	0	9.14	-9.23
0	14	0	15.03	-15.51
3	14	0	7.82	7.65
4	14	0	14.25	15.16
6	14	0	6.94	-8.09
8	14	0	7.82	-7.79
-11	0	1	4.91	4.82
-9	0	1	26.64	28.19
-7	0	1	9.49	7.87
-5	0	1	9.39	6.67
-3	0	1	6.85	-3.07
-1	0	1	65.39	66.77
1	0	1	7.25	-3.65
3	0	1	6.33	1.68
7	0	1	12.58	11.64
9	0	1	4.22	4.46
11	0	1	9.39	11.22
-12	1	1	11.53	11.26
-11	1	1	7.90	9.94
-9	1	1	13.02	14.43
-8	1	1	14.15	-15.89
-7	1	1	23.06	-24.00
-6	1	1	10.01	-11.95
-5	1	1	16.88	18.26
-4	1	1	39.58	37.28
-3	1	1	14.51	12.70
-2	1	1	8.89	13.07
-1	1	1	27.18	28.37
0	1	1	29.57	31.33
1	1	1	50.18	-47.57
2	1	1	15.93	13.20
3	1	1	12.65	-13.28
4	1	1	53.25	47.55
5	1	1	41.26	-35.03
6	1	1	3.68	4.26
7	1	1	4.04	5.34
8	1	1	16.44	-20.30
9	1	1	7.46	-9.77
10	1	1	9.67	-10.30
11	1	1	4.56	-3.55
12	1	1	10.83	8.33
-12	2	1	14.33	15.72
-11	2	1	6.77	9.12
-10	2	1	9.24	9.18
-9	2	1	10.41	-12.12
-8	2	1	25.60	-29.09
-7	2	1	5.53	-8.11
-6	2	1	29.21	30.55
-4	2	1	10.91	13.37
-3	2	1	5.23	-3.16
-2	2	1	115.30	-122.37
-1	2	1	32.55	-34.32
0	2	1	63.44	-72.76
1	2	1	43.65	-41.24
2	2	1	135.71	123.49
3	2	1	5.71	-7.15
4	2	1	3.60	-4.43
5	2	1	30.09	30.74
6	2	1	39.65	-38.49
7	2	1	4.48	-6.49
8	2	1	5.35	-6.98
9	2	1	13.54	-16.10
10	2	1	9.06	10.29
12	2	1	6.41	-8.98
14	2	1	4.38	-6.31
-12	3	1	10.29	-8.50
-10	3	1	7.46	-4.76
-9	3	1	29.47	-25.69
-8	3	1	6.59	5.91
-7	3	1	5.97	6.35
-6	3	1	24.55	23.82
-5	3	1	57.98	60.82
-4	3	1	66.27	-72.96
-3	3	1	18.20	-18.89
-2	3	1	75.69	-74.52
-1	3	1	114.18	-87.83
0	3	1	9.31	-8.79
1	3	1	42.99	43.56
2	3	1	46.28	46.29
4	3	1	63.25	-67.98
5	3	1	32.51	-33.53
7	3	1	10.63	-10.46
8	3	1	29.39	26.99
9	3	1	8.08	6.59
10	3	1	9.14	8.26
12	3	1	21.20	-19.81
-14	4	1	8.44	-7.27
-12	4	1	18.35	-13.40
-11	4	1	15.31	-16.66
-10	4	1	6.15	6.97
-9	4	1	16.80	-16.07
-8	4	1	21.54	19.43
-7	4	1	19.09	20.87
-6	4	1	23.57	-22.26
-4	4	1	4.12	-4.20
-3	4	1	44.08	-45.66
-1	4	1	29.29	-26.69
0	4	1	16.09	-10.31
1	4	1	87.56	86.36
2	4	1	45.94	-45.29
3	4	1	4.48	-4.64
4	4	1	7.12	-8.26
5	4	1	38.71	-41.11
6	4	1	34.23	33.51
8	4	1	33.69	34.01
9	4	1	23.83	21.48
10	4	1	11.03	-7.56
11	4	1	13.36	-11.43
12	4	1	6.41	-4.66
-14	5	1	3.32	-4.36
-13	5	1	13.64	-14.09
-11	5	1	5.09	-5.81
-9	5	1	19.53	17.23
-8	5	1	11.96	10.01
-7	5	1	14.59	13.11
-6	5	1	14.33	-15.84
-5	5	1	33.43	-32.39
-4	5	1	30.78	26.63
-3	5	1	6.67	-9.10
-2	5	1	49.48	41.34
-1	5	1	34.05	34.62
0	5	1	9.39	-10.51
1	5	1	39.15	34.15
2	5	1	84.79	-65.10
3	5	1	41.44	-40.48
4	5	1	24.37	23.78
5	5	1	11.85	10.06
6	5	1	16.44	15.09
7	5	1	42.67	40.28
8	5	1	3.78	-3.10
9	5	1	8.02	6.51
11	5	1	18.99	-17.57
12	5	1	15.57	14.67
13	5	1	3.78	5.08
-13	6	1	5.17	-5.09
-11	6	1	12.12	12.45
-10	6	1	5.17	-4.11
-9	6	1	13.18	14.72
-7	6	1	40.92	-37.93
-6	6	1	12.48	11.92
-4	6	1	26.04	30.13
-3	6	1	60.99	69.06
-2	6	1	2.36	2.77
-1	6	1	31.86	34.25
0	6	1	2.44	-0.08
1	6	1	35.98	-39.12
2	6	1	5.35	-4.31
3	6	1	8.70	10.79
4	6	1	6.67	9.94
5	6	1	15.75	17.06
6	6	1	6.67	-6.42
9	6	1	13.10	-15.26
12	6	1	5.17	6.99
13	6	1	6.15	7.93
-13	7	1	10.99	12.14
-12	7	1	5.53	-5.60
-11	7	1	7.38	6.48
-7	7	1	19.71	-20.75
-6	7	1	6.51	7.91
-5	7	1	20.05	20.86
-4	7	1	16.26	16.31
-3	7	1	22.34	24.35
-2	7	1	21.82	27.02
-1	7	1	26.30	-30.81
1	7	1	27.97	-32.53
2	7	1	3.68	-5.18
3	7	1	59.32	70.96
4	7	1	10.19	-9.77
6	7	1	13.46	-14.61
7	7	1	35.02	-36.76
10	7	1	5.89	5.49
11	7	1	15.57	16.45
13	7	1	8.26	-8.77
-11	8	1	13.18	-13.03
-8	8	1	7.46	-7.54
-7	8	1	33.61	29.22
-4	8	1	14.65	-13.91
-3	8	1	37.39	-39.45
-2	8	1	16.09	15.47
0	8	1	5.71	9.26
1	8	1	14.25	14.48
2	8	1	16.19	13.78
3	8	1	10.81	-9.38
4	8	1	10.55	-7.68
5	8	1	26.92	-23.60
6	8	1	13.36	-11.06
8	8	1	19.87	-17.43
9	8	1	14.41	11.64
13	8	1	8.18	-9.19
-9	9	1	11.43	8.50
-8	9	1	8.78	-6.85
-5	9	1	34.49	-34.07
-4	9	1	5.89	-4.88
-3	9	1	4.30	4.82
-2	9	1	14.77	-14.13
-1	9	1	23.93	23.60
0	9	1	4.04	-3.27
1	9	1	15.65	-13.99
2	9	1	14.85	14.82
3	9	1	12.74	-33.91
4	9	1	6.05	-5.90
5	9	1	8.78	8.42
6	9	1	4.65	-6.27
7	9	1	10.63	9.57
9	9	1	4.99	-4.18
11	9	1	7.28	-6.75
12	9	1	7.72	-7.82
-12	10	1	3.32	-4.80
-11	10	1	3.68	5.28
-10	10	1	7.56	-7.53
-7	10	1	8.08	-5.55
-6	10	1	6.94	-6.57
-4	10	1	12.72	-12.18
-3	10	1	16.70	18.78
-2	10	1	6.33	7.75
-1	10	1	13.02	-15.09
0	10	1	7.02	6.50
1	10	1	20.33	-20.26
2	10	1	8.96	-9.67
3	10	1	5.97	6.29
5	10	1	23.93	24.60
7	10	1	9.31	-10.60
9	10	1	5.61	-4.21
-11	11	1	6.23	-6.82
-9	11	1	6.33	-5.95
-7	11	1	10.37	12.12
-6	11	1	8.08	-7.40
-5	11	1	9.93	9.47
-4	11	1	8.52	-7.96
-3	11	1	10.91	-14.65
0	11	1	7.06	7.02
1	11	1	9.31	10.20
4	11	1	12.04	12.40
0	12	1	9.75	7.60
0	13	1	17.50	-15.55
0	14	1	15.39	-13.48
0	15	1	17.85	14.68
0	17	1	5.09	-4.72
-14	0	2	8.44	9.27
-12	0	2	3.60	1.49
-10	0	2	25.17	-24.99
-8	0	2	11.25	12.11
-6	0	2	58.08	52.55
-4	0	2	9.31	-8.78
-2	0	2	58.96	-56.07
0	0	2	30.44	34.03
2	0	2	39.42	39.48
4	0	2	24.63	-22.76
6	0	2	37.47	-35.86
8	0	2	19.35	20.55
10	0	2	27.62	26.65
12	0	2	8.52	-9.38
14	0	2	8.70	-13.49
-14	1	2	5.27	6.23
-13	1	2	5.89	5.85
-12	1	2	11.07	-12.87
-9	1	2	7.02	-9.34
-8	1	2	24.89	24.42
-7	1	2	21.82	17.93
-6	1	2	9.39	-1.36
-5	1	2	42.67	39.95
-4	1	2	73.92	-69.28
-3	1	2	29.73	-33.73
-2	1	2	40.04	37.39
-1	1	2	18.73	-20.71
0	1	2	92.40	90.59
1	1	2	6.05	4.78
2	1	2	52.09	-45.79
3	1	2	17.58	-17.35
4	1	2	77.62	-73.25
5	1	2	12.30	-11.54
6	1	2	26.04	25.60
7	1	2	13.97	13.36
8	1	2	21.20	20.38
10	1	2	11.60	-12.48
12	1	2	9.24	-11.10
14	1	2	4.12	6.17
-14	2	2	6.05	-7.67
-11	2	2	10.55	-10.61
-10	2	2	20.77	22.31
-7	2	2	7.02	8.69
-6	2	2	26.84	-29.02
-5	2	2	6.41	5.36
-4	2	2	11.96	-12.51
-3	2	2	8.05	-10.86
-2	2	2	30.34	32.26
-1	2	2	7.46	6.62
0	2	2	19.35	-23.70
1	2	2	27.62	32.99
2	2	2	45.22	-45.32
3	2	2	25.94	-28.06
4	2	2	4.38	2.16
5	2	2	49.62	-44.07
6	2	2	47.43	43.31
8	2	2	9.39	-9.04
9	2	2	7.90	9.44
10	2	2	20.41	-22.77
14	2	2	5.27	9.06
-13	3	2	11.43	-9.94
-9	3	2	14.85	14.94
-8	3	2	20.77	-19.71
-6	3	2	7.12	-7.25
-5	3	2	52.97	-51.46
-4	3	2	27.62	29.80
-3	3	2	14.07	10.57
-2	3	2	12.30	13.53
-1	3	2	36.96	41.29
0	3	2	59.58	-67.33
2	3	2	23.57	-24.75
3	3	2	27.54	-29.86
4	3	2	29.83	31.40
5	3	2	13.28	13.46
6	3	2	5.17	4.80
8	3	2	23.39	-23.02
9	3	2	9.06	-9.65
10	3	2	7.56	7.65
12	3	2	15.03	12.95
-14	4	2	7.02	1.59
-13	4	2	7.02	-7.45
-11	4	2	9.75	8.31
-10	4	2	12.30	-10.48
-7	4	2	21.64	-20.86
-6	4	2	13.19	10.04
-4	4	2	9.93	7.46
-3	4	2	43.65	42.02
-2	4	2	47.23	-46.72
0	4	2	10.55	9.52
1	4	2	26.66	-26.99
2	4	2	41.71	39.81
4	4	2	10.73	12.67
5	4	2	29.03	27.26
6	4	2	21.46	-17.92
7	4	2	7.12	-4.34
8	4	2	7.64	5.80
9	4	2	7.90	-7.69
10	4	2	7.90	5.25
-12	5	2	7.38	-7.56
-11	5	2	5.89	5.95
-10	5	2	7.38	9.75
-9	5	2	8.88	-8.50
-8	5	2	16.98	19.59
-7	5	2	20.67	-20.80
-5	5	2	21.82	20.52
-4	5	2	9.24	11.52
-3	5	2	28.95	31.65
-2	5	2	3.24	-2.02
-1	5	2	32.38	-28.54
0	5	2	4.56	-4.39
1	5	2	21.98	16.00
2	5	2	6.41	-6.03
3	5	2	49.80	46.23
6	5	2	9.06	-7.92
7	5	2	9.85	-9.21
8	5	2	15.75	14.86
9	5	2	10.01	9.44
10	5	2	4.65	5.14
-13	6	2	4.22	5.66
-9	6	2	6.05	8.51
-8	6	2	9.49	-11.15
-7	6	2	4.22	-5.64
-5	6	2	12.48	14.01
-4	6	2	27.79	28.28
-3	6	2	7.72	9.09
-2	6	2	31.14	33.46
-1	6	2	5.61	5.72
1	6	2	8.25	-11.28
2	6	2	8.00	-8.43
3	6	2	35.18	33.83
4	6	2	4.73	-6.46
6	6	2	6.59	-7.40
-13	7	2	5.35	7.25
-12	7	2	5.71	7.00
-10	7	2	7.02	-5.98
-8	7	2	6.59	-6.00
-6	7	2	16.09	16.40
-5	7	2	11.68	11.58
-4	7	2	8.62	10.22
-3	7	2	9.67	-11.75
-2	7	2	6.67	-8.09
-1	7	2	19.87	-21.47
0	7	2	6.33	9.71
1	7	2	9.49	-7.92
2	7	2	21.64	23.06
3	7	2	22.70	27.11
4	7	2	7.46	-9.19
5	7	2	11.35	-14.29
6	7	2	11.43	-10.60
7	7	2	13.02	-12.99
13	7	2	5.35	-8.41
-12	8	2	6.23	-6.45
-11	8	2	6.51	-6.79
-7	8	2	24.01	22.11
-5	8	2	23.39	-20.89
-4	8	2	17.42	-16.56
-3	8	2	25.50	-27.35
-2	8	2	7.38	5.95
1	8	2	29.11	29.27
3	8	2	18.81	-19.47
4	8	2	18.81	-18.22
5	8	2	18.99	-16.99
6	8	2	9.67	-10.55
7	8	2	8.00	6.79
8	8	2	12.58	-11.45
9	8	2	16.98	15.96
-9	9	2	16.70	13.62
-8	9	2	6.77	-6.19
-6	9	2	17.76	-16.98
-5	9	2	40.82	-39.03
-4	9	2	23.21	-20.12
-3	9	2	7.28	7.08
-1	9	2	49.18	38.12
0	9	2	7.28	5.73
1	9	2	27.97	-22.64
2	9	2	13.64	12.36
3	9	2	41.36	-35.80
4	9	2	9.14	-8.15
5	9	2	29.21	24.65
7	9	2	8.00	7.90
9	9	2	17.58	-16.29
11	9	2	4.22	-5.80
12	9	2	4.56	-6.33
-11	10	2	7.56	7.61
-9	10	2	9.85	-10.47
-8	10	2	9.39	9.56
-7	10	2	10.73	-10.64
-6	10	2	19.53	-19.91
-5	10	2	9.75	9.05
-3	10	2	8.08	7.17
-2	10	2	10.81	10.82
-1	10	2	25.33	-26.90
1	10	2	23.14	-22.82
2	10	2	17.76	-19.01
3	10	2	9.24	9.91
4	10	2	28.77	30.32
5	10	2	19.71	19.03
6	10	2	13.36	13.28
7	10	2	9.49	-8.34
9	10	2	6.59	-6.80
10	10	2	5.53	-7.54
11	10	2	8.08	7.69
-11	11	2	6.05	-5.74
-9	11	2	11.35	-11.62
-8	11	2	4.12	-4.77
-7	11	2	15.03	16.41
-5	11	2	17.14	18.83
-4	11	2	10.11	11.37
-3	11	2	8.44	-11.27
-2	11	2	6.94	-7.53
-1	11	2	5.09	-5.38
0	11	2	13.89	-13.40
1	11	2	27.79	26.13
3	11	2	5.79	4.44
4	11	2	22.88	24.07
5	11	2	9.75	-10.40
8	11	2	10.45	-11.27
9	11	2	11.25	13.29
11	11	2	3.94	3.80
0	13	2	25.78	21.72
0	15	2	15.47	-12.33
-11	0	3	7.46	-8.75
-9	0	3	5.79	-10.53
-7	0	3	17.50	15.67
-5	0	3	9.75	8.94
-3	0	3	9.85	-13.56
-1	0	3	18.20	-20.34
1	0	3	34.92	28.84
3	0	3	7.38	-9.49
5	0	3	12.48	-13.97
7	0	3	4.65	7.05
9	0	3	13.97	15.53
11	0	3	3.60	-3.58
-13	1	3	6.23	-7.43
-12	1	3	8.52	-8.44
-9	1	3	11.25	11.97
-5	1	3	6.67	-7.91
-3	1	3	14.33	15.68
-2	1	3	7.56	8.73
-1	1	3	24.81	24.06
0	1	3	29.47	-26.66
2	1	3	13.54	-18.84
3	1	3	9.24	-10.01
7	1	3	8.62	9.89
-13	2	3	3.60	-4.77
-11	2	3	6.59	6.80
-7	2	3	18.12	-21.96
-6	2	3	4.30	-6.58
-3	2	3	27.97	31.66
-2	2	3	21.02	23.04
-1	2	3	28.85	5.51
0	2	3	30.09	34.10
1	2	3	23.39	-27.68
2	2	3	15.21	-17.32
8	2	3	4.99	-7.99
12	2	3	10.01	11.87
-12	3	3	13.18	13.22
-11	3	3	9.31	8.18
-9	3	3	14.69	-13.61
-8	3	3	21.64	-19.71
-7	3	3	20.15	-19.90
-4	3	3	17.50	16.96
-3	3	3	28.33	28.41
-2	3	3	17.32	-17.81
-1	3	3	16.80	-17.69
1	3	3	13.36	-10.81
2	3	3	29.03	27.53
3	3	3	17.76	17.20
5	3	3	20.77	21.82
6	3	3	19.71	-17.55
7	3	3	17.42	-15.37
-13	4	3	8.62	8.50
-10	4	3	12.66	-9.09
-9	4	3	15.47	-12.94
-6	4	3	20.23	18.87
-5	4	3	30.44	32.31
-4	4	3	8.18	-8.48
-3	4	3	7.20	-5.88
-2	4	3	35.18	-33.99
-1	4	3	23.14	-24.22
1	4	3	17.76	17.20
2	4	3	33.07	32.88
3	4	3	37.91	36.78
4	4	3	27.79	-27.53
6	4	3	16.25	-15.43

Table 2 (*cont.*)

7	4	3	22.26	-20.45
8	4	3	17.06	13.94
10	4	3	5.97	5.75
11	4	3	12.40	12.41
12	4	3	9.49	-10.00
-13	5	3	4.73	5.44
-11	5	3	14.85	-14.62
-8	5	3	16.52	15.64
-7	5	3	25.07	22.24
-6	5	3	9.75	-11.45
-4	5	3	11.07	-10.38
-3	5	3	61.77	-55.01
-2	5	3	7.38	8.27
-1	5	3	9.39	9.15
0	5	3	46.20	40.56
1	5	3	56.67	53.30
2	5	3	4.48	-6.40
3	5	3	7.90	9.73
4	5	3	4.30	-4.34
5	5	3	49.18	-44.48
6	5	3	17.42	17.69
8	5	3	16.09	15.92
9	5	3	13.64	12.26
10	5	3	13.64	-13.76
11	5	3	6.77	-6.57
13	5	3	4.56	-12.08
-13	6	3	4.48	-6.93
-10	6	3	8.78	10.92
-9	6	3	20.05	20.77
-7	6	3	14.25	16.82
-6	6	3	7.38	-9.51
-5	6	3	45.94	-47.18
-4	6	3	17.86	18.32
-3	6	3	21.64	-23.92
-2	6	3	18.12	19.44
-1	6	3	51.65	52.32
0	6	3	31.50	-30.32
1	6	3	6.23	7.08
2	6	3	13.72	-13.74
3	6	3	58.08	-55.08
4	6	3	19.53	21.03
5	6	3	20.84	22.84
7	6	3	43.65	45.92
8	6	3	10.63	-11.42
9	6	3	6.41	-6.58
11	6	3	16.19	-18.55
-11	7	3	14.41	12.65
-10	7	3	7.90	-5.52
-9	7	3	12.58	10.04
-7	7	3	24.81	-25.59
-6	7	3	15.65	15.68
-4	7	3	11.96	-13.23
-3	7	3	44.44	51.78
-2	7	3	6.51	-8.63
0	7	3	11.65	-11.37
1	7	3	46.99	-52.28
2	7	3	7.02	9.60
3	7	3	4.91	4.18
4	7	3	8.15	-10.89
5	7	3	27.72	28.31
8	7	3	8.88	-9.40
9	7	3	17.24	-17.94
-12	8	3	7.72	-7.69
-9	8	3	13.80	-11.89
-8	8	3	12.74	11.07
-7	8	3	6.23	-4.93
-6	8	3	17.94	-16.71
-5	8	3	13.15	10.55
-4	8	3	7.28	-7.22
-3	8	3	9.24	-9.49
-2	8	3	16.52	15.88
-1	8	3	41.79	-36.63
0	8	3	4.91	4.18
1	8	3	12.40	-9.75
2	8	3	6.85	-5.38
3	8	3	32.02	27.97
4	8	3	6.94	6.40
5	8	3	7.20	-4.87
7	8	3	27.46	-24.76
11	8	3	9.57	8.80
-12	9	3	4.12	5.49
-11	9	3	6.77	-6.09
-9	9	3	5.35	-3.22
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-7	9	3	19.61	19.09
-6	9	3	14.77	-13.75
-5	9	3	9.31	-9.00
-4	9	3	4.73	3.39
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-1	9	3	8.52	-7.08
0	9	3	5.97	-5.36
1	9	3	14.59	10.63
2	9	3	14.51	-13.04
3	9	3	22.34	-19.63
4	9	3	11.25	9.36
7	9	3	5.71	7.22
8	9	3	9.75	-8.43
9	9	3	18.81	15.49
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-2	10	3	18.12	-16.25
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0	10	3	4.65	-4.45
2	10	3	13.80	11.43
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-8	11	3	12.22	11.78
-5	11	3	9.31	11.05
-3	11	3	10.63	-12.50
0	11	3	8.18	6.73
3	11	3	8.18	7.98
4	11	3	10.55	13.86
8	11	3	4.56	5.81
0	12	3	12.40	12.33
0	13	3	10.55	-7.19
0	14	3	6.51	-5.13
0	16	3	6.77	6.28
0	17	3	4.73	8.24
-12	0	4	3.32	5.53
-8	0	4	17.32	-15.44
-6	0	4	18.81	-17.21
-4	0	4	43.11	40.17
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0	0	4	42.31	-37.28
2	0	4	10.45	-6.73
4	0	4	43.65	42.22
8	0	4	9.93	-9.61
10	0	4	6.41	7.17
12	0	4	9.67	13.53
-10	1	4	15.21	-16.43
-7	1	4	9.85	-10.78
-6	1	4	21.64	24.21
-5	1	4	12.84	-15.71
-4	1	4	19.35	22.93
-3	1	4	15.21	15.11
-2	1	4	19.53	-20.52
0	1	4	9.93	9.28
2	1	4	27.10	26.88
3	1	4	13.46	15.25
4	1	4	13.97	15.89
5	1	4	16.52	16.29
6	1	4	31.40	-30.12
7	1	4	10.11	-9.69
8	1	4	5.61	6.16
10	1	4	14.41	14.69
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-12	2	4	6.77	-8.42
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-4	2	4	33.45	-34.88
-3	2	4	4.12	-8.35
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0	2	4	28.95	33.78
2	2	4	6.15	-7.24
3	2	4	25.17	25.49
4	2	4	41.54	-42.93
5	2	4	8.18	11.15
6	2	4	4.91	6.35
8	2	4	11.07	13.75
11	2	4	4.99	7.22
12	2	4	7.82	-9.65
-10	3	4	10.73	10.30
-7	3	4	8.26	7.68
-6	3	4	26.35	-24.65
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-2	3	4	41.44	38.00
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0	3	4	11.17	-9.60
1	3	4	10.63	8.53
2	3	4	27.28	-26.86
3	3	4	16.70	-14.90
4	3	4	22.85	20.88
5	3	4	42.49	-37.79
6	3	4	21.25	17.03
7	3	4	11.53	8.88
8	3	4	14.07	-12.95
10	3	4	8.08	-8.66
-12	4	4	9.14	8.53
-9	4	4	12.22	9.73
-8	4	4	12.30	-12.06
-6	4	4	15.57	14.41
-5	4	4	48.84	-47.01
-4	4	4	21.25	21.47
-2	4	4	24.27	-21.75
-1	4	4	20.84	21.38
0	4	4	16.88	-15.19
1	4	4	18.81	-17.63
2	4	4	29.47	27.17
3	4	4	18.73	-16.79
4	4	4	17.58	15.72
5	4	4	28.67	27.12
6	4	4	17.68	-16.82
8	4	4	10.63	-10.16
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-11	5	4	6.51	7.50
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0	5	4	13.54	11.23
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2	5	4	9.05	9.65
3	5	4	4.22	-4.73
4	5	4	21.64	-21.63
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7	5	4	5.27	5.79
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4	6	4	14.51	15.97
5	6	4	9.06	-8.60
6	6	4	12.30	13.16
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-4	7	4	21.10	22.33
-1	7	4	24.99	-28.24
0	7	4	17.86	-18.55
1	7	4	7.56	-7.48
2	7	4	8.70	-5.06
3	7	4	14.51	14.22
4	7	4	17.14	16.26
5	7	4	15.13	14.91
7	7	4	7.72	-7.95
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-4	8	4	8.52	-8.38
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0	8	4	6.05	-5.70
1	8	4	27.46	26.34
3	8	4	8.12	9.86
4	8	4	8.18	-7.26
5	8	4	26.38	-26.01
9	8	4	19.82	19.35
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-9	9	4	8.00	6.70
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-6	9	4	8.08	7.77
-5	9	4	17.92	-14.38
-3	9	4	11.53	-10.50
-2	9	4	12.04	-11.30
-1	9	4	27.10	24.06
0	9	4	11.53	10.46
1	9	4	6.94	4.52
2	9	4	11.07	10.27
3	9	4	18.12	-18.20
4	9	4	5.71	-6.37
5	9	4	15.57	-14.35
7	9	4	9.49	9.87
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1	10	4	17.76	-16.27
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3	10	4	13.89	-13.28
4	10	4	9.55	-9.59
5	10	4	14.85	14.79
7	10	4	5.09	5.75
8	10	4	7.12	7.21
9	10	4	6.15	-6.55
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-3	11	4	11.96	12.22
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3	11	4	9.39	11.81
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0	12	4	15.65	-12.94
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0	14	4	9.24	6.34
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7	0	5	13.25	-14.04
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-2	2	5	9.14	11.43
-1	2	5	10.37	10.05
0	2	5	25.60	27.42
2	2	5	4.30	-6.09
3	2	5	9.57	-7.75
4	2	5	5.53	-6.41
5	2	5	8.15	-10.42
8	2	5	6.41	8.86
10	2	5	3.65	-5.02
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7	3	5	15.31	13.36
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10	4	5	9.75	9.56
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1	5	5	6.85	6.27
2	5	5	4.65	6.08
3	5	5	19.35	17.14
4	5	5	7.38	-7.28
5	5	5	8.08	-8.94
7	5	5	23.65	-24.52
8	5	5	7.72	9.23
9	5	5	8.70	10.92
-10	6	5	4.30	3.87
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2	6	5	9.67	-10.53
3	6	5	11.17	-13.46
5	6	5	12.48	-15.03
6	6	5	6.33	7.37
7	6	5	9.14	10.63
9	6	5	11.60	13.12
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-2	7	5	7.82	-9.39
-1	7	5	29.21	28.99
3	7	5	15.31	-15.52
4	7	5	7.20	6.28
7	7	5	16.09	16.13
9	7	5	8.26	-9.53
-8	8	5	9.85	9.43
-7	8	5	13.36	-12.28
-6	8	5	8.34	7.89
-4	8	5	6.85	-6.87
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1	8	5	20.77	-17.24
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6	9	5	4.91	5.81
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-1	2	6	5.09	7.92
1	2	6	19.87	-23.10
2	2	6	15.65	17.35
3	2	6	3.94	4.83
4	2	6	7.82	-8.57
5	2	6	8.70	10.83
6	2	6	12.22	-13.81
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0	3	6	9.24	9.66
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4	3	6	7.28	-7.43
6	3	6	10.01	8.78
7	3	6	8.08	-6.83
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2	5	6	9.14	8.72
3	5	6	5.53	-6.84
6	5	6	7.38	-7.46
-8	6	6	6.94	7.97
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-1	6	6	10.55	12.86
0	6	6	27.18	26.89
3	6	6	4.91	-5.43
4	6	6	7.90	-9.05
5	6	6	4.48	2.92
8	6	6	5.89	9.23
-7	7	6	5.09	-5.15
-6	7	6	9.31	-10.05
-2	7	6	9.06	8.07
-1	7	6	9.93	10.60
6	7	6	8.08	7.73
-8	8	6	6.33	-5.47
-4	8	6	12.40	10.47
-2	8	6	7.02	6.19
0	8	6	15.31	-14.16
3	8	6	9.75	9.15
4	8	6	5.79	7.29
-6	9	6	8.15	7.23
-5	9	6	6.33	5.60
-3	9	6	4.99	-7.03
-2	9	6	7.82	-8.52
-1	9	6	10.29	-8.70
0	9	6	7.20	-9.41
1	9	6	6.77	8.36
2	9	6	8.18	8.01
5	9	6	4.99	-5.70
-6	10	6	3.42	4.20
-5	10	6	4.04	-4.86
-3	10	6	5.71	-6.82
-2	10	6	8.00	-8.42
1	10	6	6.23	7.23
2	10	6	4.65	5.54
3	10	6	5.09	-6.18
5	10	6	5.79	-5.91
-5	11	6	6.59	-7.73
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0	11	6	7.72	10.91
1	11	6	5.89	-6.89
3	11	6	3.94	-5.97
4	11	6	3.16	-6.35
-7	0	7	21.82	-18.32
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1	0	7	20.23	-20.28
3	0	7	7.72	7.67
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-5	1	7	14.15	14.71
-4	1	7	9.49	9.09
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3	1	7	16.09	17.71
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0	2	7	6.59	8.00
1	2	7	9.31	11.89
2	2	7	12.58	14.15
4	2	7	8.52	-10.81
5	2	7	8.70	-10.72
6	2	7	6.85	-8.92
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1	3	7	6.51	6.52
3	3	7	11.96	-10.93
4	3	7	8.05	-7.04
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6	3	7	6.41	6.21
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-2	4	7	8.96	8.29
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2	4	7	11.25	-10.41
3	4	7	11.60	-12.52
5	4	7	9.57	10.18
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1	5	7	9.24	-11.26
4	5	7	6.15	5.90
5	5	7	7.38	8.14
-5	6	7	5.89	7.05
-1	6	7	3.78	-4.13
0	6	7	3.65	6.46
3	6	7	8.62	10.67
-3	7	7	9.85	-9.95
0	7	7	4.65	-4.99
1	7	7	10.29	12.41
5	7	7	4.35	-6.18
-1	8	7	9.67	9.51
0	8	7	7.38	-7.32
2	8	7	6.67	6.74
3	8	7	7.02	-7.73
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-2	9	7	3.50	-5.75
-1	9	7	8.78	-10.08
0	9	7	5.45	6.39
1	9	7	5.53	-5.89
-4	0	8	9.39	-10.48
0	0	8	11.60	12.53
2	0	8	4.99	-6.86
-2	1	8	6.23	7.48
2	1	8	6.67	-8.32
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-1	2	8	9.31	11.47
0	2	8	4.30	-6.73
2	2	8	4.22	6.04
3	2	8	4.12	-6.54
-4	3	8	5.79	-6.85
-3	3	8	8.18	7.03
-2	3	8	5.09	-4.75
-1	3	8	6.15	6.09
1	3	8	8.70	-9.61
2	3	8	6.77	5.23
-2	4	8	8.00	7.54
-1	4	8	11.86	-11.14
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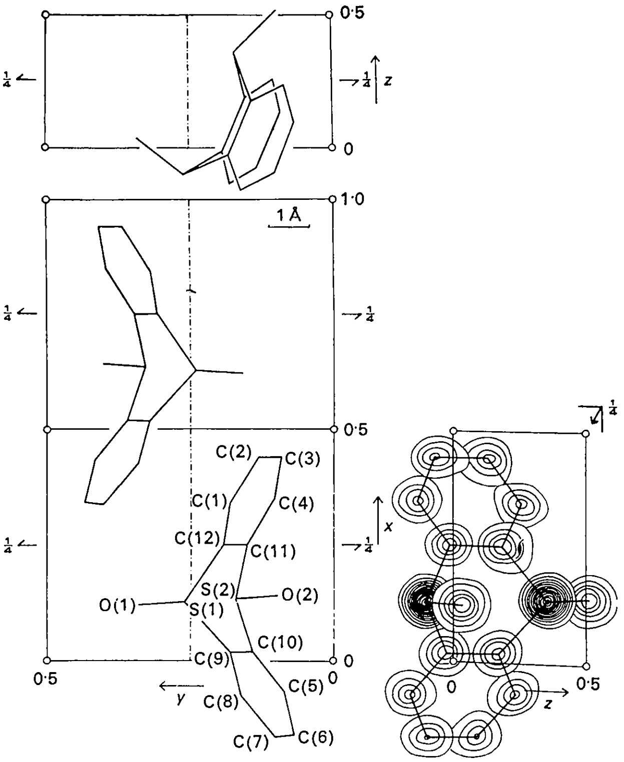

Fig. 3. Projected view of β-thianthrene dioxide. Contour interval of the three-dimensional Fourier map is 1 e.Å^{-3} beginning at 1 e.Å^{-3}.

$|F_o|$ on different layers were brought into common scale with $hk0$ reflexions. Because the agreement between $|F_o|$ and $|F_c|$ of three-dimensional data was found to be reasonably good, a cycle of three-dimensional least-squares refinement was carried out on the DEUCE computer in the National Physical Laboratory, London, with the program devised by Rollett. The shifts obtained by this calculation proved later to bring R for the observed reflexions down from 26·6% to 19·1%. More cycles of three-dimensional refinement were carried out on the IBM 7090 computer with the program ORFLS, which was devised by Busing, Martin & Levy (1962) and modified by Iitaka so as to refine parameters successively one group after another. After three cycles of refinement, R for 1293 observed terms decreased to 10·7%. In this computation, an equal weight was given to each reflexion, and the refining was carried out on $|F|$. Hydrogen atoms were entirely neglected. The final parameters, fractional coordinates and anisotropic temperature parameters are shown in Table 1 with their standard deviations. The values of F_c thus obtained are compared with $|F_o|$ values in Table 2. The three-dimensional Fourier map for each atom is shown as a part of Fig. 3. This synthesis was computed on a CDC G-20 machine with the program devised by Sakurai.

Molecular dimensions

Bond lengths and bond angles among atoms in a molecule were obtained as shown in Table 3. According

Table 3. *Bond lengths and angles with standard deviations*

Bond	Length	Standard deviation (× 10³ Å)
S(1)—O(1)	1·479 Å	16
S(2)—O(2)	1·474	16
S(1)—C(12)	1·828	22
S(1)—C(9)	1·753	21
S(2)—C(11)	1·720	21
S(2)—C(10)	1·866	21
C(12)-C(11)	1·429	30
C(9)—C(10)	1·431	28
C(12)-C(1)	1·324	31
C(9)—C(8)	1·433	29
C(11)-C(4)	1·400	32
C(10)-C(5)	1·329	30
C(1)—C(2)	1·397	35
C(8)—C(7)	1·404	32
C(4)—C(3)	1·379	36
C(5)—C(6)	1·465	33
C(2)—C(3)	1·450	37
C(7)—C(6)	1·358	34

Bonds	Angle	Standard deviation
O(1) -S(1)—C(12)	103·18°	0·01°
O(1) -S(1)—C(9)	108·18	0·01
O(2) -S(2)—C(11)	106·27	0·01
O(2) -S(2)—C(10)	109·66	0·01
C(12)-S(1)—C(9)	96·75	0·02
C(11)-S(2)—C(10)	95·72	0·02
S(2)—S(1)—O(1)	74·36	0·01
S(1)—S(2)—O(2)	157·66	0·01
S(1)—C(12)-C(11)	122·22	0·02
S(1)—C(9)—C(10)	119·53	0·02
S(2)—C(11)-C(12)	120·03	0·03
S(2)—C(10)-C(9)	121·34	0·02
S(1)—C(12)-C(1)	118·84	0·03
S(1)—C(9)—C(8)	118·41	0·02
S(2)—C(11)-C(4)	116·61	0·03
S(2)—C(10)-C(5)	118·92	0·02
C(11)-C(12)-C(1)	118·94	0·03
C(10)-C(9)—C(8)	121·97	0·03
C(12)-C(11)-C(4)	123·13	0·03
C(9)—C(10)-C(5)	119·61	0·03
C(12)-C(1)—C(2)	120·81	0·04
C(9)—C(8)—C(7)	118·26	0·03
C(11)-C(4)—C(3)	117·18	0·04
C(10)-C(5)—C(6)	117·66	0·03
C(1)—C(2)—C(3)	120·40	0·04
C(8)—C(7)—C(6)	117·85	0·04
C(4)—C(3)—C(2)	119·48	0·04
C(5)—C(6)—C(7)	124·64	0·04

to data so far accumulated (Abrahams, 1956), a sulphur–carbon distance is about 1·61 Å in the double-bond case, and about 1·82 Å in the single-bond case. The distances found in four S–C bonds in the present compound imply that they have mostly double-bond character. As for the S–O bond length, there has been much discussion about the character of this bond. It is now considered that the double-bond length is 1·43–1·44 Å, and that a standard single-bond length may be 1·60 Å (Abrahams, 1956). Therefore the bond in the present compound may be nearly double-bonded, though the percentage double-bond character cannot be estimated.

The C–S–C bond angles have been found to be 96–97°, which is a typical value found in various compounds as discussed previously (Hosoya, 1958*c*, 1963).

The best planes were calculated for two benzene rings in relation to the molecule having the bond-length and bond-angle values shown in Table 3. They are expressed by the following equations:

$$0{\cdot}34200X+0{\cdot}92207Y+0{\cdot}18118Z=3{\cdot}8536$$
[for C(1), C(2), C(3), C(4), C(11) and C(12)],

$$-0{\cdot}44412X+0{\cdot}87779Y+0{\cdot}17945Z=6{\cdot}8615$$
[for C(5), C(6), C(7), C(8), C(9) and C(10)].

The distances of atoms from the best planes are listed in Table 4. Coplanarity of carbon atoms making each benzene ring is fairly good, while both sulphur atoms lie slightly outside the dihedral angle made by the two benzene rings. The dihedral angle was found to be 133°38′.

Table 4. *Distances of atoms from the best planes*

First benzene ring		Second benzene ring	
C(1)	−0·0122 Å	C(5)	−0·0050 Å
C(2)	0·0040	C(6)	0·0049
C(3)	0·0022	C(7)	−0·0010
C(4)	−0·0026	C(8)	−0·0040
C(11)	−0·0054	C(9)	0·0039
C(12)	0·0117	C(10)	−0·0004
S(1)	0·0713	S(1)	0·1146
S(2)	0·1164	S(2)	0·1176
O(1)	1·3542	O(1)	1·3972
O(2)	−0·3620	O(2)	−0·3908

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A Modified *N*(*z*) Test for Crystal Symmetry

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A modified $N(z)$ test for distinguishing between the centric and acentric distributions is described. It can be performed as quickly and as easily as the standard $N(z)$ test and offers better discrimination.

Introduction

Wilson (1949) showed that the probability distributions of the intensities of X-ray reflexions from crystals are different for centrosymmetric and non-centrosymmetric crystals. The two distributions – known respectively as the centric and acentric distributions – are uniquely determined if the unit of crystal pattern contains a reasonably large number of approximately equal atoms distributed at random. Several practical tests have been devised for distinguishing between the distributions (*International Tables for X-ray Crystallography*, 1959). The one which has been most widely used in practice, as an aid to space-group determination, is