Acta Cryst. (1962). **15**, 410

The Crystal Structure of $B_{10}H_{12}[S(CH_3)_2]_2$.*

By Donald E. Sands

Lawrence Radiation Laboratory, University of California, Livermore, California, U.S.A.

and Allan Zalkin

Lawrence Radiation Laboratory, University of California, Berkeley, California, U.S.A.

(*Received* 22 *June* 1961)

$B_{10}H_{12}[S(CH_3)_2]_2$ is monoclinic with

$$a=11\cdot83,\ b=10\cdot78,\ c=12\cdot74\ \text{Å};\ \beta=95\cdot17°;$$

the space group is $P2_1/c$ and there are four molecules per unit cell. The symmetry of the decaborane skeleton is retained in this derivative, but the four hydrogen bridges of decaborane are replaced by two bridges at positions 5, 10 and 7, 8. The substituent groups are attached to the 6, 9 positions. The structural details conform closely to those of $B_{10}H_{12}(CH_3CN)_2$.

Introduction

The structure of the decaborane derivative, $B_{10}H_{12}(CH_3CN)_2$, has been reported by Reddy & Lipscomb (1959). The interesting molecular features of this compound and the unusual interpretation given them in terms of the topological theory of boron hydrides have prompted the determination of the structure of a derivative involving a different electron donor. Since the molecules in crystals of $B_{10}H_{12}[S(CH_3)_2]_2$ lie in general positions with all atoms crystallographically independent, this structure provides a rigorous test of the molecular symmetry unconstrained by the crystal lattice.

Experimental

Oscillation and Weissenberg photographs of single crystals of $B_{10}H_{12}[S(CH_3)_2]_2$, taken with Cu $K\alpha$ radiation ($\lambda=1\cdot5418$ Å), revealed a monoclinic unit cell with

$$a=11\cdot83\pm0\cdot02,\ b=10\cdot78\pm0\cdot02,\ c=12\cdot74\pm0\cdot02\ \text{Å};\ \beta=95\cdot17\pm0\cdot10°.$$

The space group indicated by the systematic extinctions is C_{2h}^5–$P2_1/c$; four molecules per unit cell give a calculated density of 1·032 g.cm.$^{-3}$. A crystal used in this investigation had the approximate dimensions $0\cdot3\times0\cdot2\times0\cdot1$ mm., with the c-axis of the monoclinic cell parallel to the longest edge.

Triple film Weissenberg exposures of the $l=0$ through the $l=9$ layers of a c-axis oriented crystal were taken with Cu $K\alpha$ radiation. A second crystal, oriented about the b-axis, was used for the $h0l$ and $h1l$ layers. The intensities of 987 independent reflections, of which 328 were too weak to be observed, were obtained from these films by visual comparison with a standard scale. After correction for the Lorentz, polarization, and velocity factors these data were placed on the same scale by cross-correlating the layers from the two crystals.

Although these visually estimated intensities proved adequate for determining approximate parameters for the sulfur, carbon, and boron atoms, attempts to refine these parameters and to locate the hydrogen atoms indicated the need for better data. A crystal was mounted on a General Electric XRD-5 X-ray spectrometer equipped with a single-crystal orienter. The intensities of all reflections with $2\theta \geq 150°$ were measured with Cu $K\alpha$ radiation using the stationary crystal-stationary counter technique and a krypton-filled proportional counter. The settings were made for the $K\alpha_1$ position ($\lambda=1\cdot54050$ Å), and an empirical correction for the α_1–α_2 dispersion was made (Tulinsky, Worthington & Pignataro, 1959). Forty-second counts were taken on all reflections. Background corrections were obtained from a plot of intensity versus angle made with the crystal out of reflecting position. The intensities of 3330 independent reflections, of which 1502 were not observable above background, were recorded.

The crystal decomposed on exposure to X-rays, manifested by a steady decrease in the diffracted intensities to about one-third of their initial values after 100 hours of exposure. The intensities of all reflections apparently decreased at the same rate, so a correction for this decay was obtained by monitoring a few standard reflections. An additional phenomenon was the appearance, after exposure to X-rays, of a diffuse spot along the ($h00$) row at $2\theta=27\cdot9°$. This spot, which was also observed on the photographs, increased in intensity at a decreasing rate until it was approximately one-tenth as strong as (200)—the strongest reflection present.

---

* This work was performed under the auspices of the U.S. Atomic Energy Commission.

Determination of the structure

Analysis of the three-dimensional Patterson function

computed from the photographic data established that the sulfur atoms occupy two sets of general positions of space group $P2_1/c$: $\pm(x, y, z; x, \frac{1}{2}-y, \frac{1}{2}+z)$

Table 1. *Observed and calculated structure factors*, FO *and* FC, *respectively*

Values are multiplied by 10. Asterisks denote unobserved reflections

H	K	FO	FC
	L=-16		
1	0*	29	-23
	L=-15		
1	1*	39	-44
2	1*	39	-47
3	1*	38	10
4	1*	37	15
5	1*	34	-5
6	1*	30	-15
1	2*	38	-12
2	2*	38	70
3	2*	37	-9
4	2	35	-68
5	2*	33	18
1	3*	36	-23
2	3*	36	3
3	3*	35	6
4	3*	33	-9
5	3*	30	-3
1	4*	33	-20
2	4*	32	-2
3	4*	31	17
	L=-14		
1	0	45	-71
2	0*	45	-18
3	0	44	59
4	0	44	49
5	0*	43	-43
6	0*	40	-20
7	0	51	59
8	0*	31	10
1	1*	45	-30
2	1	63	-62
3	1*	44	36
4	1	87	64
5	1*	42	-33
6	1*	40	-36
7	1*	36	23
8	1*	30	19
1	2*	44	30
2	2*	44	-38
3	2*	44	-20
4	2*	43	55
5	2*	42	21
6	2*	39	-36
7	2*	34	-21
1	3*	43	-42
2	3*	43	13
3	3	43	45
4	3*	42	-11
5	3*	40	-46
6	3*	36	11
7	3*	32	30
1	4*	42	-2
2	4	59	50
3	4*	41	10
4	4*	39	-34
5	4*	37	12
6	4*	33	35
1	5*	38	-28
2	5	38	-19
3	5*	37	16
4	5*	35	15
5	5*	32	-9
1	6*	33	-43
2	6*	33	42
3	6*	31	25
4	6*	29	-36
	L=-13		
1	1	124	142
2	1	47	31
3	1	81	-74
4	1*	46	9
5	1*	45	57
6	1*	44	-26
7	1	43	-77
8	1*	39	11
9	1*	34	45
1	2*	47	35
2	2*	46	-16
3	2	46	20
4	2*	46	8
5	2*	45	-26
6	2*	44	-14
7	2*	42	3
8	2*	38	6
9	2*	32	-12
1	3*	46	-40
2	3*	46	16
3	3*	46	62
4	3*	45	-23
5	3*	44	-43
6	3*	43	-10
7	3*	40	11
8	3*	36	22
9	3*	29	-9
1	4*	45	-15
2	4	111	-113
3	4*	45	22
4	4	77	90
5	4*	43	-40
6	4	41	-67
7	4*	37	45
8	4	32	59
1	5*	44	24
2	5*	44	-4
3	5*	43	0
4	5*	42	-2
5	5*	41	-2
6	5*	37	-8
7	5*	33	-21
1	6*	41	33
2	6*	41	70
3	6*	40	-20
4	6	67	-54
5	6*	36	-5
6	6	32	34
1	7	36	-49
2	7*	36	23
3	7*	34	69
4	7	32	-9
5	7	50	-60
	L=-12		
1	0*	47	-52
2	0	106	113
3	0	67	68
4	0	105	-107
5	0	47	-52
6	0	47	52
7	0*	46	17
8	0*	44	-7
9	0	41	-11
10	0*	35	12
1	1*	47	33
2	1	82	-109
3	1*	47	-57
4	1	67	59
5	1*	47	46
6	1	66	-62
7	1*	46	-21
8	1	76	75
9	1*	41	22
10	1	35	-36
1	2	82	90
2	2*	47	15
3	2	116	-114
4	2*	47	-25
5	2	47	61
6	2	46	-6
7	2*	45	-34
8	2*	43	27
9	2	40	45
10	2*	33	8
1	3	82	104
2	3*	47	4
3	3	67	-80
4	3*	47	-9
5	3	46	60
6	3*	46	-20
7	3*	44	-34
8	3*	42	33
9	3*	38	10
10	3*	30	-15
1	4	81	-65
2	4	47	-31
3	4	47	51
4	4	80	47
5	4	46	-73
6	4	63	-54
7	4	106	80
8	4*	40	33
9	4	60	-44
1	5	46	41
2	5	46	25
3	5*	46	-8
4	5*	45	-19
5	5*	45	16
6	5	43	25
7	5*	41	-18
8	5*	36	-15
9	5*	29	1
1	6*	45	-21
2	6	63	-64
3	6*	44	37
4	6	44	44
5	6*	43	-45
6	6*	40	-49
7	6*	36	36
8	6	53	44
1	7*	43	-22
2	7	104	-75
3	7*	42	25
4	7*	40	21
5	7*	38	-26
6	7*	34	-12
7	7*	29	11
1	8	37	40
2	8*	37	-28
3	8	36	-36
5	8*	30	16
	L=-11		
1	1	46	-36
2	1*	47	22
3	1*	47	-1
4	1*	47	-34
5	1*	47	-25
6	1*	47	66
7	1*	47	29
8	1	80	-63
9	1*	44	8
10	1*	41	39
11	1*	34	-30
1	2*	47	14
2	2	169	164
3	2	82	-72
4	2	47	-95
5	2	47	69
6	2	82	72
7	2	81	-28
8	2*	46	-64
9	2	44	6
10	2*	40	27
11	2*	33	-9
1	3	82	-94
2	3*	47	-2
3	3	116	117
4	3	47	61
5	3	116	-86
6	3*	47	15
7	3	93	76
8	3*	45	-41
9	3	74	-58
10	3*	38	-13
11	3*	30	17
1	4	47	28
2	4*	47	-9
3	4*	47	-44
4	4*	47	-10
5	4*	47	57
6	4	81	16
7	4	46	-56
8	4	44	8
9	4	41	36
10	4*	35	-6
1	5	188	195
2	5*	47	-55
3	5	176	-167
4	5*	47	46
5	5	93	96
6	5*	46	-15
7	5	44	-53
8	5*	42	7
9	5	37	47
10	5*	30	-2
1	6	47	-12
2	6	47	68
3	6*	46	27
4	6	79	-76
5	6*	45	-27
6	6*	44	55
7	6*	42	8
8	6*	38	-34
9	6*	32	-15
1	7*	45	-5
2	7*	45	-21
3	7*	45	10
4	7*	44	41
5	7*	43	-3
6	7*	41	-42
7	7	37	18
8	7*	32	28
1	8	129	-91
2	8	74	-67
3	8	73	65
4	8	41	68
5	8*	38	-44
6	8*	35	-42
7	8	51	52
1	9*	37	-19
2	9*	36	18
3	9	35	22
4	9*	33	-9
5	9*	29	5
	L=-10		
1	0	334	-327
2	0	249	-219
3	0	268	269
4	0	236	222
5	0	191	-176
6	0	115	-116
7	0	134	143
8	0	67	38
9	0	92	-104
10	0	63	-74
11	0	41	34
12	0	65	69
1	1	108	-87
2	1	133	-127
3	1	110	90
4	1	144	111
5	1	46	-29
6	1*	47	-20
7	1*	47	2
8	1*	47	12
9	1*	46	6
10	1*	44	-34
11	1*	40	-4
12	1	32	16
1	2*	45	49
2	2*	45	-51
3	2*	45	-8
4	2*	46	-12
5	2*	47	-9
6	2	47	43
7	2*	47	-27
8	2	66	-39
9	2	46	34
10	2*	44	19
11	2*	39	-2
12	2	30	0
1	3*	46	-47
2	3	158	144
3	3*	46	55
4	3	114	-121
5	3	47	-51
6	3	116	123
7	3*	47	-20
8	3	104	-102
9	3	45	32
10	3	43	52
11	3*	37	-10
1	4	46	71
2	4	47	10
3	4*	47	-17
4	4*	47	-32
5	4*	47	27
6	4*	47	16
7	4	94	-78
8	4	46	-11
9	4	44	41
10	4*	41	-5
11	4*	34	2
1	5	47	-44
2	5*	47	13
3	5*	47	9
4	5*	47	12
5	5*	47	6
6	5*	47	2
7	5*	46	-17
8	5*	45	-19
9	5*	42	9
10	5*	37	18
1	6*	47	-24
2	6	67	47
3	6*	47	-8
4	6*	47	-24
5	6	66	55
6	6*	46	29
7	6	45	-43
8	6*	43	-22
9	6*	39	13
10	6*	32	-5
1	7	81	49
2	7	105	-88
3	7	47	-45
4	7	113	105
5	7	64	56
6	7	44	-57
7	7*	42	-47
8	7*	38	24
9	7*	32	24
1	8	111	108
2	8	45	39
3	8	90	-77
4	8*	44	-43
5	8	43	52
6	8*	41	27
7	8*	37	-58
8	8	44	-28
1	9	42	56
2	9*	42	26
3	9*	41	-19
4	9	40	9
5	9*	37	-5
6	9*	33	3
1	10	60	-66
2	10*	34	2
3	10	81	103
4	10*	30	4
	L= -9		
1	1	41	18
2	1	71	-72
3	1	73	-99
4	1*	43	18
5	1	44	73
6	1*	46	-17
7	1*	47	5
8	1*	47	18
9	1*	47	-19
10	1*	46	-9
11	1*	44	31
12	1*	38	14
1	2	144	-148
2	2	103	82
3	2	252	241
4	2	44	-59
5	2	246	-219
6	2*	46	24
7	2	82	95
8	2*	47	-35
9	2	66	-60
10	2	46	37
11	2	105	70
12	2*	37	-14
1	3	254	-249
2	3*	43	13
3	3	44	36
4	3	45	-38
5	3*	46	36
6	3*	47	-17
7	3*	47	32
8	3	47	32
9	3	47	-51
10	3*	45	-4
11	3*	42	15
12	3*	34	1
1	4	172	-168
2	4	264	-265
3	4	111	111
4	4	220	238
5	4*	47	-31
6	4	125	-125
7	4*	47	39
8	4	81	84
9	4	46	-21
10	4	76	-70
11	4*	39	1
12	4	30	31
1	5	46	-38
2	5	113	114
3	5	81	-60
4	5	163	-173
5	5	82	83
6	5	125	131
7	5*	47	-52
8	5	80	-60
9	5	45	39
10	5*	42	46
11	5*	35	-17
1	6*	47	-24
2	6	116	108
3	6	47	40
4	6*	47	-35
5	6*	47	-50
6	6	47	20
7	6*	46	19
8	6*	45	-32
9	6*	43	-4
10	6*	38	20
11	6*	29	21
1	7	116	-123
2	7*	47	23
3	7	105	110
4	7*	47	-20
5	7	81	-77
6	7*	46	22
7	7*	45	17
8	7*	43	-14
9	7*	38	-2
10	7*	31	-0
1	8	93	87
2	8	47	9
3	8	80	-57
4	8*	46	33
5	8	78	64
6	8*	44	-41
7	8	42	-78
8	8*	37	22
9	8	31	40
1	9*	45	6
2	9*	45	-44
3	9*	44	-33
4	9*	43	16
5	9*	42	22
6	9*	39	-12
7	9*	35	-12
1	10	71	25
2	10	40	-1
3	10*	39	-27
4	10*	37	-2
5	10	34	52
6	10*	30	3
1	11	31	61
2	11	30	-31
	L= -8		
1	0	74	68
2	0	129	141
3	0	94	-128
4	0	40	37
5	0	171	195
6	0	75	-76
7	0	120	-123
8	0	47	10
9	0*	47	9
10	0*	47	-7
11	0*	45	-2
12	0*	42	12
13	0*	34	8
1	1	105	103
2	1	232	-234
3	1	232	-226
4	1	155	170
5	1	200	204
6	1	107	-124
7	1*	46	-70
8	1	105	101
9	1*	47	27
10	1	81	-48
11	1	45	-45
12	1*	42	-2
13	1	33	20
1	2	191	199
2	2*	39	-6
3	2	331	-325
4	2*	41	2
5	2	307	293
6	2	44	27
7	2	122	-119
8	2*	47	-15
9	2*	47	62
10	2	47	-1
11	2	45	-62
12	2*	41	-1
13	2*	32	19
1	3*	40	11
2	3	40	24
3	3	41	-17
4	3*	42	18
5	3	62	-61
6	3	45	-43
7	3	104	103
8	3	47	6
9	3	94	-69
10	3	65	23
11	3*	44	49
12	3*	39	-16
13	3*	29	-29
1	4	138	-133
2	4*	42	-6
3	4	60	56
4	4	76	67
5	4*	45	-22
6	4*	46	-3
7	4	47	63
8	4	47	-37
9	4	47	-38
10	4*	45	11
11	4*	43	-11
12	4*	36	4
1	5	107	76
2	5	76	27
3	5*	45	-21
4	5	79	76
5	5*	46	-25
6	5	67	-56
7	5*	47	14
8	5*	47	-17
9	5	46	-9
10	5*	44	2
11	5*	40	16
12	5*	31	11
1	6	220	-218
2	6*	46	-27
3	6	213	194
4	6	81	68
5	6	134	-135
6	6	47	-33
7	6	67	100
8	6*	46	7
9	6	63	-82
10	6*	42	-11
11	6*	35	46
1	7*	47	-13
2	7	47	34
3	7	67	-71
4	7	47	-41
5	7	47	72
6	7	47	27
7	7*	46	-21
8	7	45	-10
9	7*	42	20
10	7*	37	18
1	8*	47	21
2	8*	47	8
3	8*	47	-28
4	8	46	-33
5	8	46	41
6	8	79	65
7	8	44	-18
8	8*	42	-25
9	8*	36	3
1	9	103	-62
2	9	185	168
3	9*	46	33
4	9	143	-141
5	9*	44	-20
6	9	43	73
7	9*	40	19
8	9*	35	-47
1	10	44	-30
2	10	44	-45
3	10*	43	12
4	10	72	76
5	10*	39	-4
6	10	36	-41
7	10*	31	12
1	11	37	-8
2	11*	36	-32
3	11*	35	9
4	11	32	47
	L= -7		
1	1	131	139
2	1	207	198
3	1*	35	19
4	1	264	-246
5	1*	39	11
6	1	83	77
7	1	76	-65
8	1*	46	9
9	1*	47	44
10	1*	47	24
11	1	46	-19
12	1*	44	-22
13	1*	38	8
1	2	277	258
2	2*	35	-3
3	2	284	-261
4	2	54	44
5	2	105	105
6	2*	42	-36
7	2*	44	-26
8	2*	46	-15
9	2*	47	42
10	2*	47	2
11	2	65	-46
12	2*	43	18
13	2*	36	15
1	3*	36	-37
2	3	74	-74
3	3	298	316
4	3	223	228
5	3	226	-226
6	3	225	-196
7	3	45	53
8	3	66	66
9	3*	47	-58
10	3*	47	-60
11	3	45	62
12	3	42	57
13	3*	34	-15
1	4	299	269
2	4	146	-147
3	4	327	-336
4	4	131	121
5	4	243	266
6	4	127	-101
7	4	139	-135
8	4	47	63
9	4	94	77
10	4*	46	-41
11	4	63	-63
12	4*	40	17
13	4*	30	29
1	5	270	261
2	5	59	-86
3	5	141	-143
4	5*	44	8
5	5*	45	37
6	5*	46	14
7	5*	47	-24
8	5*	47	5
9	5	47	16
10	5*	45	2
11	5*	43	8
12	5*	36	-16
1	6	98	-78
2	6*	44	46
3	6	63	61
4	6	112	-111
5	6	123	-99
6	6*	47	66
7	6	82	86
8	6*	47	-34
9	6*	46	-36
10	6*	44	18
11	6*	39	8
12	6*	30	-4
1	7*	46	-11
2	7	66	-92
3	7	47	50
4	7*	47	96
5	7	67	-77
6	7	47	-89
7	7	66	55
7	7*	47	55
9	7	44	-45
10	7*	41	-14
11	7	33	35
1	8	47	-59
2	8	106	-88
3	8*	47	24
4	8	47	73
5	8*	47	-35
6	8*	47	-8
7	8	64	54
8	8*	44	-28
9	8*	40	-14
10	8*	34	2
1	9	47	45
2	9	47	42
3	9*	47	-32
4	9	46	23
5	9	46	33
6	9	45	-11
7	9	43	-35
8	9*	39	-72
9	9*	33	10
1	10	64	-58
2	10*	45	-74
3	10*	45	34
4	10	44	14
5	10	43	-49
6	10*	40	-3
7	10	62	51
8	10*	29	-5
1	11	41	32
2	11	81	82
3	11	39	-36
4	11	75	-73
5	11*	34	30
6	11*	30	69
1	12	31	0
2	12*	30	20
	L= -6		
1	0	367	-357
2	0	31	-42
3	0	463	468
4	0*	34	10
5	0	376	-407
6	0	86	-93
7	0	272	247
8	0	63	62
9	0	131	-117
10	0*	47	6
11	0*	47	26
12	0*	45	-15
13	0*	41	5
14	0*	31	6
1	1	43	27
2	1	31	-26
3	1	46	-54
4	1	119	119
5	1	196	218
6	1*	39	-26
7	1	156	-136
8	1*	44	-10
9	1	47	59
10	1*	47	-35
11	1*	47	-41
12	1*	45	29
13	1*	41	31
14	1*	31	3
1	2	152	149
2	2	238	263
3	2	47	-27
4	2	468	-474
5	2	65	-52
6	2	221	238
7	2	42	42
8	2*	45	-13
9	2*	47	16
10	2	67	70
11	2*	47	-11
12	2	118	-87
13	2*	40	4
1	3	116	-98
2	3	184	206
3	3	35	36
4	3	278	-285
5	3*	39	3
6	3	184	155
7	3*	44	-3
8	3	46	-48
9	3*	47	18
10	3*	47	2
11	3*	46	-18
12	3*	44	17
13	3*	38	5
1	4	119	129
2	4	115	-84
3	4	37	-19
4	4	103	-90
5	4	41	-64
6	4	43	-58
7	4	45	8
8	4	155	132
9	4*	47	3
10	4*	47	-29
11	4*	45	25
12	4*	42	-22
13	4*	34	-13
1	5	102	-87
2	5	110	116
3	5	40	29
4	5	238	-225
5	5*	43	-11
6	5	135	129
7	5	80	58
8	5*	47	-34
9	5*	47	-32
10	5	46	32
11	5*	44	-3
12	5*	39	-17
13	5*	29	2
1	6	239	237
2	6	126	-110
3	6	231	-236
4	6	139	136
5	6	170	136
6	6	114	-108
7	6*	47	-59
8	6	67	62
9	6	47	50
10	6*	45	-30
11	6*	42	-42
12	6*	34	6
1	7*	45	-11
2	7	193	-193
4	7	122	121
5	7	47	54
6	7	67	-71
7	7*	47	-7
8	7	47	46
9	7*	45	-25
10	7*	43	-42
11	7*	37	3
1	8	105	115
2	8*	47	50
3	8	170	-162
4	8	82	-79
5	8*	47	60
6	8	47	42
7	8	46	-8
8	8*	45	-19
9	8*	43	27
10	8*	38	20
21	8*	29	-14
1	9	67	-89
2	9	47	-43
3	9	141	131
4	9	66	-32
5	9	154	-138
6	9	65	57
7	9	77	95
8	9	42	-21
9	9	37	-61
1	10	131	-136
2	10	80	-49
3	10	112	111
4	10	45	18
5	10	99	-101
6	10*	43	-28
7	10	39	57
8	10	34	21
1	11	62	60
2	11	75	-81
3	11	60	-60
4	11*	41	30
5	11	38	39
6	11*	34	1
1	12	35	-38
2	12	49	11
3	12	33	14
4	12*	30	-18
	L= -5		
1	1*	27	4
2	1	369	-336
3	1	51	67
4	1	190	195
5	1	127	-121
6	1	52	34
7	1	105	95
8	1*	43	-7
9	1	46	-42
10	1*	47	-40
11	1*	47	-11
12	1*	46	1
13	1*	43	12
14	1*	34	5
1	2	445	-427
2	2	317	306
3	2	515	519
4	2	430	-442
5	2	398	-376
6	2	168	180
7	2	135	143
8	2	44	-25
9	2	65	-71
10	2*	47	44
11	2	94	68
12	2*	45	-26
13	2*	42	-26
14	2*	32	-7
1	3	102	-68
2	3	180	-172
3	3	33	15
4	3	189	193
5	3	97	-99
6	3	96	-108
7	3	103	97
8	3	63	65
9	3*	47	-41
10	3	67	-40
11	3	47	-31
12	3*	45	12
13	3*	40	19
14	3	29	-12
1	4	58	-76
2	4	34	11
3	4	50	-48
4	4*	37	5
5	4	226	217
6	4	41	36
7	4	98	-87
8	4*	46	-47
9	4*	47	-1
10	4*	47	19
11	4	80	-40
12	4*	44	-9
13	4	37	39
1	5	96	98
2	5	320	319
3	5	196	-209
4	5	249	-263
5	5	222	217
6	5	213	203
7	5	79	-71
8	5	105	-94
9	5*	47	56
10	5	47	33
11	5	78	-68
12	5*	42	-23
13	5	33	33
1	6	97	-92
2	6	120	125
3	6*	41	53
4	6	141	-151
5	6	44	-31
6	6*	46	56
7	6	47	52
8	6*	47	-5
9	6*	47	-41
10	6*	46	18
11	6*	43	10
12	6*	37	-6
1	7	61	-63
2	7*	43	-38
3	7	44	48
4	7	90	56
5	7*	46	-10
6	7*	47	-34
7	7*	47	-5
8	7*	47	23
9	7*	46	25
10	7	44	-45
11	7*	40	-28
12	7	43	32
1	8	178	164
2	8	122	-117
3	8	104	-125
4	8*	47	39
5	8	125	116
6	8	47	-75
7	8	94	-91
8	8	79	80
9	8*	44	29
10	8	40	-29
11	8*	33	-1
1	9*	47	-33
2	9*	47	20
3	9	47	-7
4	9*	47	-23
5	9	47	-7
6	9	46	46
7	9	64	51
8	9*	44	-33
9	9*	40	-17
10	9*	33	19
1	10	94	94
2	10	47	-32
3	10	147	-127
4	10	46	19
5	10	157	136
6	10*	44	-13
7	10	59	-77
8	10*	37	19
9	10	43	26
1	11	63	-38
2	11	45	-12
3	11	44	11
4	11*	43	-2
5	11*	41	-2
6	11*	38	2
7	11*	33	35
1	12	67	-72
2	12	54	43
3	12	37	43
4	12*	34	-39
5	12	30	-34
	L= -4		
1	0	435	443
2	0	573	-521
3	0	305	298
4	0	623	633
5	0	190	-211
6	0	373	-359
7	0	169	-215
8	0	149	144
9	0	118	110
10	0	115	-111
11	0*	47	51
12	0	46	88
13	0*	44	-15
14	0*	37	-33
1	1	141	173
2	1	184	-179
3	1	229	-242
4	1	242	218
5	1	187	168
6	1	121	-126
7	1	38	-32
8	1	59	47
9	1	45	-41
10	1*	47	-8
11	1*	47	-12
12	1	46	-7
13	1*	44	6
14	1*	36	-7
1	2*	26	57
2	2	53	97
3	2*	28	2
4	2	53	18
5	2	81	97
6	2	176	191
7	2	103	-115
8	2	169	-174
9	2	45	23
10	2*	47	34
11	2*	47	26
12	2*	46	-0
13	2*	43	-16
14	2*	35	21
1	3	349	-298
2	3	29	-44
3	3	405	376
4	3	56	-56
5	3	299	-302
6	3	37	-10
7	3	134	171
8	3	44	26
9	3	172	-111
10	3	47	41
11	3	67	61
12	3*	45	-32
13	3*	42	-26
14	3*	32	-0
1	4	170	-155
2	4	179	175
3	4	171	170
4	4	35	5
5	4	83	-52
6	4	69	88
7	4*	42	-32
8	4	149	-127
9	4*	47	29
10	4*	47	15
11	4	47	-12
12	4	45	31
13	4*	39	7
1	5	59	65
2	5	163	-182
3	5	204	212
4	5	141	119
5	5	164	-163
6	5	103	-108
7	5*	44	-20
8	5	66	69
9	5*	47	4
10	5	67	-43
11	5	46	30
12	5*	43	26
13	5*	35	-18
1	6	276	-263
2	6	127	132
3	6	371	350
4	6	91	-74
5	6	275	-253
6	6*	45	21
7	6	80	61
8	6*	47	-47
9	6*	47	-20
10	6	46	16
11	6	44	36
12	6*	39	20
13	6*	29	-17
1	7	194	200
2	7	84	92
3	7	201	-182
4	7*	44	-2
5	7	143	140
6	7	47	-4
7	7	82	-99
8	7*	47	8
9	7	66	56
10	7*	45	-1
11	7	42	-31
12	7*	33	-4
1	8*	45	9
2	8	192	199
3	8*	46	5
4	8	174	-174
5	8*	47	64
6	8	67	105
7	8*	47	-41
8	8	81	-64
9	8*	45	3
10	8*	42	30
11	8*	35	-7
1	9	31	-74
2	9	163	165
3	9*	47	38
4	9	67	-84
5	9*	47	-34
6	9	47	-3
7	9	46	27
8	9	44	22
9	9*	42	-11
10	9*	35	-9
1	10*	47	11
2	10	125	-129
3	10	47	7
4	10	162	136
5	10	46	9
6	10	100	-119
7	10*	43	-4
8	10	40	58
9	10*	33	-4
1	11	91	87
2	11*	45	-9
3	11	64	-61
4	11	44	41
5	11	43	52
6	11*	40	-32
7	11	36	-54
8	11*	29	8
1	12	101	108
2	12*	41	-3
3	12	68	-72
4	12	37	13
5	12	34	41
1	13	42	-33
	L= -3		
1	1	176	-85
2	1	487	493
3	1	472	-469
4	1	61	-129
5	1	416	419
6	1	34	-25
7	1	196	-213
8	1*	41	34
9	1	108	112
10	1*	46	16
11	1*	47	-12
12	1*	47	-9
13	1*	44	-7
14	1*	37	-12
1	2	184	199
2	2	333	-322
3	2	37	-26
4	2	170	153
5	2	45	-51
6	2	85	-49
7	2	53	45
8	2	41	46
9	2*	45	-13
10	2*	47	-15
11	2*	47	10
12	2	46	-9
13	2*	44	-18
14	2*	36	18
1	3	151	148
2	3	270	-269
3	3	176	164
4	3	353	351
5	3	47	-54
6	3	237	-267
7	3	142	-201
8	3	74	77
9	3	164	147
10	3*	47	-29
11	3*	47	17
12	3*	46	41
13	3*	43	-10
14	3*	34	-17
1	4	784	730
2	4	259	-265
3	4	284	-270
4	4	331	343
5	4	163	154
6	4	199	-213
7	4	155	-209
8	4	108	115
9	4	139	127
10	4	47	-31
11	4*	47	-29
12	4	45	-9
13	4*	40	9
14	4*	30	5
1	5	187	-191
2	5	156	150

Table 1 (*cont.*)

H	K	FO	FC
3	5	60	66
4	5	178	-175
5	5	54	-37
6	5	148	136
7	5	44	47
8	5	46	-71
9	5	47	-44
10	5	41	65
11	5*	46	44
12	5	44	-42
13	5*	37	-35
1	6	130	-117
2	6	133	124
3	6	298	291
4	6	143	-158
5	6	274	-245
6	6	87	74
7	6*	46	59
8	6*	47	15
9	6*	47	-20
10	6*	47	13
11	6*	45	52
12	6	41	-36
13	6*	31	-31
1	7	208	-219
2	7	108	-118
3	7	110	124
4	7*	43	29
5	7	77	-80
6	7	80	-97
7	7	47	66
8	7	67	75
9	7	47	-46
10	7*	45	9
11	7*	42	25
12	7*	35	-10
1	8	98	85
2	8	183	159
3	8*	45	32
4	8	92	-104
5	8*	47	-12
6	8	95	101
7	8	47	-53
8	8*	47	-62
9	8	45	52
10	8*	43	24
11	8*	37	-16
1	9	81	80
2	9*	47	7
3	9*	47	-8
4	9*	47	-30
5	9*	47	4
6	9	47	-28
7	9	46	-34
8	9*	45	23
9	9*	43	17
10	9*	37	2
1	10*	47	3
2	10	106	105
3	10	47	46
4	10	66	-51
5	10	66	-78
6	10*	45	26
7	10*	44	27
8	10*	41	-27
9	10*	35	9
1	11	80	82
2	11	103	103
3	11	79	-72
4	11	110	-105
5	11	44	43
6	11	42	49
7	11*	37	-27
8	11*	31	-4
1	12	43	-32
2	12*	42	6
3	12	58	59
4	12*	39	-1
5	12	36	-53
6	12	31	-21
1	13	46	-9
2	13	44	-36
3	13	29	-1
L= -2			
1	0	680	-676
2	0	314	326
3	0	70	74
4	0	279	187
5	0	122	-185
6	0	79	-58
7	0	124	178
8	0	105	-127
9	0	61	-58
10	0*	46	34
11	0*	47	-1
12	0*	47	17
13	0*	45	-26
14	0*	39	-4
1	1	1308	1258
2	1	78	46
3	1	446	-481
4	1	341	317
5	1	391	406
6	1	33	-62
7	1	351	-380
8	1	40	-69
9	1	213	221
10	1*	46	2
11	1	67	-80
12	1*	47	15
13	1*	44	50
14	1*	38	8
1	2	488	-389
2	2	517	501
3	2	281	-273
4	2	47	10
5	2	188	158
6	2	34	20
7	2	74	113
8	2	81	-62
9	2	76	-60
10	2	47	34
11	2*	47	-1
12	2	47	-15
13	2*	44	-20
14	2*	37	-13
1	3	93	100
2	3	67	-52
3	3	54	-31
4	3	142	129
5	3	72	-79
6	3	71	-87
7	3*	39	-22
8	3	59	108
9	3*	45	38
10	3	94	-88
11	3*	47	8
12	3*	46	27
13	3*	43	-7
14	3*	35	-9
1	4	189	-192
2	4	263	-247
3	4	30	-45
4	4	262	238
5	4	35	36
6	4	231	-230
7	4*	41	58
8	4	124	125
9	4	46	-59
10	4*	47	-19
11	4*	47	24
12	4*	45	-11
13	4*	41	-14
14	4*	31	-4
1	5	44	-22
2	5	78	76
3	5	88	-119
4	5*	35	-49
5	5	53	51
6	5	40	-2
7	5*	43	-3
8	5	79	86
9	5*	47	26
10	5	47	-33
11	5*	46	-26
12	5*	44	-14
13	5	37	16
1	6	172	180
2	6	403	-430
3	6	83	-92
4	6	394	374
5	6	115	112
6	6	211	-201
7	6*	45	-29
8	6*	47	99
9	6*	47	-4
10	6	47	-46
11	6*	45	-16
12	6*	41	15
13	6*	32	3
1	7	103	125
2	7	89	-93
3	7	41	-3
4	7	127	136
5	7	44	-19
6	7	79	-76
7	7*	47	-35
8	7*	47	-1
9	7*	47	36
10	7*	46	12
11	7*	43	-14
12	7*	36	-12
1	8	75	55
2	8	97	82
3	8	77	-89
4	8	45	-55
5	8	66	67
6	8	82	68
7	8*	47	10
8	8	47	-38
9	8*	46	-16
10	8	43	34
11	8*	38	-7
1	9	207	-220
2	9*	46	-18
3	9	162	237
4	9*	47	-14
5	9	171	-197
6	9	47	10
7	9	66	107
8	9	45	2
9	9*	43	-41
10	9*	38	5
11	9	41	23
1	10	47	-41
2	10	82	-74
3	10*	47	23
4	10	47	24
5	10	47	18
6	10	65	-29
7	10*	44	-29
8	10	42	54
9	10*	36	15
1	11	46	44
2	11	46	-25
3	11	65	-48
4	11*	45	-3
5	11	44	37
6	11*	42	-10
7	11*	39	-10
8	11*	33	12
1	12	43	-6
2	12	114	117
3	12*	42	14
4	12	98	-120
5	12*	37	10
6	12	80	107
1	13	34	27
2	13	33	30
3	13*	31	-24
L= -1			
1	1	223	348
2	1	266	244
3	1	117	124
4	1	87	-106
5	1	107	-136
6	1	158	181
7	1	95	109
8	1	247	-246
9	1	75	-55
10	1	113	113
11	1*	47	14
12	1*	47	-33
13	1*	45	-4
14	1*	38	40
1	2	815	-732
2	2	409	398
3	2	172	171
4	2	429	-423
5	2	184	-187
6	2	156	131
7	2	82	108
8	2	40	34
9	2	44	-41
10	2	46	-15
11	2*	47	36
12	2*	47	-8
13	2*	44	-15
14	2*	37	-13
1	3*	23	29
2	3	378	-370
3	3	26	-12
4	3	161	161
5	3	90	-98
6	3	171	-157
7	3	54	82
8	3	102	86
9	3*	45	-35
10	3*	47	-35
11	3*	47	-14
12	3*	46	18
13	3*	43	3
14	3*	35	-1
1	4	327	306
2	4	425	399
3	4	256	-268
4	4	127	-91
5	4	128	113
6	4	219	242
7	4	90	-71
8	4	242	-260
9	4	46	34
10	4	82	73
11	4*	47	-26
12	4*	45	-6
13	4*	41	8
14	4*	31	13
1	5	483	423
2	5	351	328
3	5	263	-292
4	5	60	-83
5	5	193	197
6	5	56	80
7	5	60	-58
8	5	90	-97
9	5*	47	1
10	5*	47	39
11	5*	46	-12
12	5*	44	-7
13	5*	38	18
1	6	356	-337
2	6	35	-50
3	6	121	114
4	6	132	142
5	6	198	-208
6	6*	43	-23
7	6	201	211
8	6*	47	-36
9	6	106	-90
10	6*	47	-13
11	6*	45	28
12	6	42	26
13	6*	32	-22
1	7	237	224
2	7	207	-210
3	7*	40	-38
4	7	229	238
5	7*	44	22
6	7	144	-148
7	7	94	-93
8	7	47	64
9	7	47	37
10	7	46	-54
11	7*	43	1
12	7	36	32
1	8*	43	16
2	8	173	-185
3	8	76	-86
4	8	135	133
5	8*	46	24
6	8	115	-88
7	8*	47	19
8	8	47	30
9	8*	46	-3
10	8	44	-7
11	8*	38	-7
1	9	46	-31
2	9	46	-37
3	9	93	87
4	9	47	13
5	9	67	-53
6	9*	47	29
7	9	47	5
8	9*	45	0
9	9*	43	-12
10	9*	38	-13
11	9*	29	10
1	10*	47	38
2	10	116	-121
3	10	47	-31
4	10	105	105
5	10	47	25
6	10*	46	-39
7	10*	45	7
8	10*	42	-4
9	10*	37	-10
1	11	93	-96
2	11	46	47
3	11	92	104
4	11*	45	-16
5	11	44	-67
6	11*	43	24
7	11	39	37
8	11	33	-34
1	12	76	-84
2	12	43	29
3	12	42	49
4	12	41	-14
5	12	38	-33
6	12*	33	11
1	13*	35	-21
2	13	34	-65
3	13	32	34
L= 0			
1	0	119	109
2	0	1653	-1914
3	0	51	17
4	0	151	196
5	0	49	-44
6	0	480	-514
7	0	50	-0
8	0	459	488
9	0	61	54
10	0	172	-147
11	0*	47	-24
12	0	47	30
13	0*	45	31
14	0*	38	-28
1	1	47	-54
2	1	91	66
3	1	43	-73
4	1	43	-46
5	1*	29	27
6	1	120	141
7	1*	36	-8
8	1	131	-140
9	1*	43	-1
10	1	80	59
11	1	47	-23
12	1*	47	-22
13	1*	44	2
14	1*	38	10
0	2	592	466
1	2	76	-69
2	2	74	8
3	2*	23	29
4	2	363	-375
5	2*	30	-40
6	2	185	182
7	2	110	148
8	2	70	-51
9	2	88	-77
10	2	47	46
11	2*	47	-4
12	2*	47	-26
13	2*	44	22
14	2*	36	15
1	3	763	-617
2	3	41	45
3	3	91	100
4	3	58	-59
5	3	55	-48
6	3	116	129
7	3	148	129
8	3	94	-113
9	3	45	-35
10	3	47	46
11	3*	47	-2
12	3*	46	1
13	3*	43	2
14	3*	34	3
0	4	295	239
1	4	170	141
2	4	61	-52
3	4	88	-83
4	4	95	-82
5	4*	34	-24
6	4	52	55
7	4*	40	42
8	4*	44	-2
9	4*	46	-8
10	4*	47	-12
11	4*	47	-9
12	4*	45	21
13	4*	41	9
14	4*	30	-11
1	5	230	-208
2	5	44	14
3	5*	33	34
4	5*	35	-11
5	5	37	29
6	5	69	100
7	5*	43	-25
8	5	128	-142
9	5*	47	16
10	5	47	42
11	5*	46	14
12	5*	44	1
13	5*	37	-9
0	6	118	146
1	6	113	78
2	6	121	98
3	6	73	-68
4	6	305	-307
5	6*	40	-15
6	6	128	111
7	6	78	-82
8	6*	47	32
9	6	67	78
10	6*	47	4
11	6*	45	-14
12	6*	41	-18
13	6*	32	12
1	7	348	296
2	7	141	-112
3	7	317	-297
4	7	72	92
5	7	227	223
6	7	45	42
7	7	132	-135
8	7*	47	-48
9	7	81	81
10	7*	46	-15
11	7	43	-40
12	7*	36	28
0	8	264	-260
1	8	60	10
2	8	251	218
3	8	62	36
4	8	202	-190
5	8	80	-70
6	8	141	144
7	8*	47	34
8	8	81	-70
9	8	46	-31
10	8*	43	33
11	8	38	32
1	9	152	-128
2	9	65	-72
3	9	47	15
4	9	67	78
5	9*	47	10
6	9*	47	-51
7	9*	47	32
8	9	45	30
9	9	43	-31
10	9	38	-26
0	10	150	147
1	10	67	21
2	10	171	-165
3	10*	47	2
4	10	133	144
5	10	47	-44
6	10*	46	-75
7	10*	45	8
8	10*	42	18
9	10*	36	9
1	11	155	120
2	11	66	-7
3	11	122	-101
4	11*	45	-2
5	11	117	105
6	11*	43	18
7	11	78	-81
8	11*	33	-23
0	12	62	38
1	12*	44	3
2	12	61	-30
3	12*	43	18
4	12	41	21
5	12	53	-43
6	12*	33	-15
1	13	87	-78
2	13*	34	-23
3	13	55	79
L= 1			
0	1	102	-125
1	1	327	-420
2	1	89	-88
3	1	231	-269
4	1	160	-139
5	1	177	145
6	1	65	80
7	1	89	155
8	1	40	62
9	1	116	-118
10	1	46	-49
11	1*	47	-32
12	1	47	12
13	1*	44	23
14	1*	37	-20
0	2	184	163
1	2	963	-871
2	2	358	-393
3	2	222	263
4	2	456	475
5	2	142	-102
6	2	216	-210
7	2	204	219
8	2	41	33
9	2	154	-134
10	2	47	-34
11	2*	47	37
12	2	46	39
13	2*	43	-16
14	2*	35	-7
0	3	813	698
1	3	40	29
2	3	265	-244
3	3	60	-68
4	3	211	-220
5	3	116	105
6	3*	35	45
7	3	55	-69
8	3	73	64
9	3	45	34
10	3*	47	-32
11	3*	47	-20
12	3*	46	1
13	3*	42	16
14	3*	33	-1
0	4	845	781
1	4	153	157
2	4	307	-292
3	4	107	-110
4	4	150	154
5	4	139	158
6	4	119	-125
7	4	82	-109
8	4*	44	44
9	4	66	58
10	4*	47	-4
11	4*	47	-10
12	4*	45	7
13	4*	40	4
0	5	498	-458
1	5	517	-446
2	5	341	322
3	5	239	230
4	5	337	-354
5	5	159	-158
6	5	332	348
7	5	149	170
8	5	177	-167
9	5	94	-88
10	5	47	57
11	5	46	6
12	5	43	-37
13	5*	36	-5
0	6	141	130
1	6	464	-455
2	6	61	-49
3	6	160	155
4	6*	38	-3
5	6*	41	13
6	6	43	-79
7	6	45	42
8	6	66	83
9	6	47	-59
10	6	47	-30
11	6	45	32
12	6*	40	17
13	6	30	-7
0	7	132	140
1	7	185	-159
2	7	104	-106
3	7	41	-41
4	7	60	50
5	7	44	26
6	7*	46	3
7	7	47	41
8	7*	47	17
9	7*	47	5
10	7*	45	-13
11	7*	42	-34
12	7*	35	1
0	8	232	-233
1	8*	43	2
2	8	189	198
3	8	88	-106
4	8	101	-95
5	8	161	165
6	8	47	55
7	8	67	-58
8	8	66	-41
9	8*	46	-16
10	8*	43	10
11	8*	37	11
0	9*	46	-9
1	9*	46	17
2	9*	46	29
3	9	47	-44
4	9*	47	-22
5	9	47	31
6	9*	47	27
7	9	47	-17
8	9*	45	-20
9	9*	43	18
10	9*	37	7
0	10	95	-88
1	10	47	51
2	10	95	79
3	10	47	-61
4	10	94	-82
5	10	66	63
6	10	46	46
7	10	44	-54
8	10*	42	-16
9	10*	36	22
0	11	47	-47
1	11	93	87
2	11	46	-24
3	11	80	-71
4	11	78	48
5	11*	44	27
6	11*	42	-9
7	11*	38	-9
8	11*	32	10
0	12	62	49
1	12	107	-97
2	12	43	-44
3	12	73	74
4	12*	40	20
5	12	37	-34
6	12*	33	-23
0	13	71	71
1	13	35	21
2	13	75	-84
3	13	31	-39
L= 2			
0	0	853	-924
1	0	762	736
2	0	232	184
3	0	274	-274
4	0	116	-47
5	0	333	339
6	0	33	43
7	0	287	-335
8	0*	41	-29
9	0	133	117
10	0	47	-42
11	0*	47	-45
12	0	80	56
13	0*	43	28
14	0*	35	-10
0	1	67	262
1	1	1081	1049
2	1	91	94
3	1	158	-162
4	1	148	-105
5	1	179	157
6	1*	34	-4
7	1	221	-223
8	1	41	-19
9	1	118	110
10	1	47	15
11	1*	47	-5
12	1*	46	2
13	1*	43	-0
14	1*	35	4
0	2	897	-829
1	2	354	289
2	2	388	380
3	2	210	219
4	2	153	-152
5	2	44	-46
6	2	177	204
7	2	76	-75
8	2	126	-113
9	2*	45	8
10	2*	47	10
11	2*	47	16
12	2*	46	12
13	2*	43	-7
14	2*	33	-2
0	3	189	164
1	3	81	-49
2	3	178	-174
3	3*	28	-13
4	3	110	92
5	3*	33	-35
6	3	167	-163
7	3	40	66
8	3	105	93
9	3	65	-58
10	3*	47	-26
11	3	47	20
12	3*	45	5
13	3*	41	-14
14	3*	31	-3
0	4	177	214
1	4	104	88
2	4	178	-188
3	4	31	44
4	4	109	120
5	4*	36	20
6	4	67	-54
7	4	83	-113
8	4*	45	17
9	4	66	64
10	4*	47	-19
11	4*	47	-21
12	4*	44	8
13	4*	38	20
0	5	44	38
1	5	83	-96
2	5	32	-35
3	5	148	-176
4	5	88	108
5	5	108	122
6	5	136	-158
7	5	44	78
8	5	92	92
9	5	67	-61
10	5*	47	-14
11	5*	46	-26
12	5*	43	8
13	5*	34	14
0	6	231	256
1	6	264	-248
2	6	226	-200
3	6	176	191
4	6	272	255
5	6	93	-73
6	6	116	-117
7	6*	46	45
8	6*	47	18
9	6*	47	-42
10	6	46	-43
11	6*	44	20
12	6*	39	35
0	7	165	-136
1	7	111	90
2	7	289	275
3	7	41	-23
4	7	242	-249
5	7	44	43
6	7	103	112
7	7	67	-42
8	7	95	-101
9	7	47	8
10	7	64	85
11	7*	41	-2
12	7*	33	-41
0	8	192	-195
1	8	75	-59
2	8	152	143
3	8	45	63
4	8*	46	-3
5	8	66	-68
6	8	47	45
7	8	47	42
8	8	93	-77
9	8*	45	-5
10	8*	42	15
11	8*	35	-2
0	9	46	-44
1	9	167	-188
2	9	66	43
3	9	124	144
4	9*	47	-37
5	9	82	-97
6	9	47	15
7	9	65	59
8	9*	45	-1
9	9*	42	-31
10	9*	35	8
0	10	82	72
1	10	67	59
2	10	47	-28
3	10	47	-78
4	10	47	47
5	10	66	74
6	10	79	-51
7	10	44	-51
8	10*	40	27
9	10	34	28
0	11	93	-65
1	11	93	72
2	11	65	57
3	11	79	-84
4	11	45	-36
5	11*	44	48
6	11*	41	29
7	11	37	-13
8	11*	30	-18
0	12	157	-146
1	12*	43	-20
2	12	142	138
3	12	42	4
4	12	78	-81
5	12*	36	20
6	12	31	45
0	13	34	24
1	13	34	34
2	13*	32	-25
3	13	30	-19
L= 3			
0	1	658	-553
1	1	166	117
2	1	472	522
3	1	615	540
4	1	330	-324
5	1	282	-274
6	1	127	127
7	1	55	-98
8	1*	42	-41
9	1	64	68
10	1	47	46
11	1	47	71
12	1	46	-27
13	1*	42	-47
14	1*	32	8
0	2	85	-52
1	2	203	216
2	2	50	43
3	2	216	-214
4	2	100	-129
5	2	119	99
6	2*	36	-25
7	2*	40	-2
8	2	74	93
9	2*	46	12
10	2*	47	-17
11	2*	47	-18
12	2*	45	-10
13	2*	41	7
14	2*	30	-6
0	3	280	298
1	3	26	-16
2	3	117	-159
3	3	172	-158
4	3	157	154
5	3	92	109
6	3	206	-237
7	3	92	-100
8	3	182	193
9	3	46	56
10	3	67	-49
11	3	47	-5
12	3*	45	4
13	3*	39	-2
0	4	221	-199
1	4	658	635
2	4	191	253
3	4	250	-227
4	4	271	-283
5	4	184	188
6	4	112	131
7	4	142	-153
8	4*	45	-41
9	4	82	58
10	4*	47	10
11	4*	46	-27
12	4*	43	2
13	4*	36	10
0	5	214	-198
1	5	93	88
2	5	89	128
3	5	137	160
4	5	37	36
5	5	137	-146
6	5	73	-80
7	5	45	32
8	5	47	31
9	5*	47	-20
10	5	47	-3
11	5*	45	54
12	5*	41	10
13	5*	31	-31
0	6	173	170
1	6	51	-73
2	6	124	-190
3	6	155	172
4	6	107	119
5	6	181	-186
6	6	77	-84
7	6	114	118
8	6*	47	74
9	6*	47	-34
10	6	46	-42
11	6	43	-0
12	6*	37	19
0	7	226	223
1	7	235	220
2	7	101	-155
3	7	95	-76
4	7	107	112
5	7*	45	11
6	7	132	-126
7	7	67	-76
8	7	47	62
9	7	80	51
10	7*	44	-23
11	7*	39	10
12	7*	30	12
0	8	205	196
1	8	116	105
2	8	77	-106
3	8	45	-8
4	8*	46	9
5	8	47	-48
6	8*	47	-15
7	8*	47	7
8	8	46	26
9	8	44	26
10	8*	41	3
11	8*	32	-22
0	9	47	19
1	9	47	-71
2	9*	47	25
3	9*	47	-26
4	9*	47	-22
5	9*	47	23
6	9	47	-24
7	9*	46	7
8	9*	44	24
9	9*	40	2
10	9*	33	-6
0	10	116	115
1	10*	47	-23
2	10	47	-68
3	10	81	84
4	10*	47	20
5	10	65	-68
6	10*	45	-7
7	10*	43	22
8	10	38	19
9	10*	31	-10
0	11	113	-111
1	11*	46	-56
2	11	112	143
3	11*	45	22
4	11	99	-111
5	11*	43	-17
5	11	69	56
7	11*	35	17
0	12	43	-4
1	12*	43	-3
2	12	42	-21
3	12*	40	12
4	12	53	38
5	12*	34	-33
0	13	33	45
1	13	32	30
2	13	30	-16
L= 4			
0	0	391	448
1	0	169	-178
2	0	274	-256
3	0	306	-281
4	0	194	178
5	0	34	39
6	0	137	-187
7	0	40	42
8	0	130	137
9	0*	46	32
10	0*	47	28
11	0*	47	-30
12	0	78	-87
13	0*	40	6
0	1	142	-163
1	1	173	172
2	1	458	428
3	1	243	-227
4	1	439	-417
5	1	204	194
6	1	209	223
7	1	90	-104
8	1	98	-94
9	1*	46	33
10	1	47	59
11	1	47	-39
12	1	45	-43
13	1*	40	23
0	2	561	-520
1	2	182	-197
2	2	136	139
3	2	190	172
4	2	45	55
5	2	201	-174
6	2	38	17
7	2	92	102
8	2*	44	-26
9	2*	47	-30
10	2*	47	21
11	2	47	3
12	2	44	-32
13	2	38	-7
0	3*	28	-32
1	3	255	-237
2	3	73	74
3	3	192	203
4	3	144	-129
5	3	73	-72
6	3	97	75
7	3	43	51
8	3*	45	13
9	3	47	-27
10	3*	47	1
11	3*	46	5
12	3*	43	-8
13	3*	36	2
0	4	291	-272
1	4	177	177
2	4	65	72
3	4	149	-119
4	4	63	74
5	4	39	27
6	4	41	-43
7	4*	44	20
8	4*	46	9
9	4*	47	5
10	4*	47	4
11	4*	45	-6
12	4*	42	-10
13	4*	33	-15
0	5	113	-111
1	5	77	101
2	5	36	121
3	5	138	173
4	5	194	-196
5	5	117	-134
6	5	131	143
7	5*	46	11
8	5*	47	-54
9	5*	47	-7
10	5	46	27
11	5*	44	25
12	5*	38	-26
0	6*	38	-38
1	6	243	264
2	6*	39	46
3	6	380	-385
4	6	59	-63
5	6	256	246
6	6	46	-49
7	6	66	-71
8	6	82	62
9	6	66	48
10	6*	45	12
11	6*	42	-36
12	6*	33	-26
0	7	274	200
1	7	118	142
2	7	127	-90
3	7	44	-31
4	7*	45	-52
5	7*	46	10
6	7*	47	32
7	7*	47	-12
8	7	81	50
9	7*	46	-5
10	7*	43	-29
11	7*	37	6
0	8	118	-137
1	8	119	-110
2	8	112	101
3	8	92	97
4	8	94	-92
5	8	47	-42
6	8	47	48
7	8	94	67
8	8*	46	-10
9	8	43	-55
10	8	38	9
0	9	176	187
1	9	82	-89
2	9	164	-159
3	9	67	81
4	9	116	113
5	9	81	-84
6	9	80	-88
7	9	45	73
8	9	74	68
9	9	38	-37
10	9*	29	-33
0	10	156	154
1	10*	47	-25
2	10	176	-146
3	10	47	-12
4	10	103	87
5	10*	45	23
6	10	62	-46
7	10*	41	1
8	10	36	28
0	11	46	-15
1	11	64	75
2	11	45	45
3	11*	44	-19
4	11	43	-42
5	11*	41	-10
6	11*	37	26
7	11*	32	-2
0	12*	42	23
1	12	82	-97
2	12	56	-17
3	12	53	55
4	12*	35	-9
5	12	43	-44
0	13	30	2
1	13	29	-37
L= 5			
0	1	152	105
1	1	74	-98
2	1	330	-322
3	1	113	95
4	1	368	388
5	1	115	-122
6	1	111	-113
7	1	85	109
8	1*	45	4
9	1	66	-50
10	1*	47	-46
11	1*	46	-17
12	1*	43	33
13	1	36	15
0	2	29	22
1	2	346	-337
2	2	328	-312
3	2	315	332
4	2	299	318
5	2	232	-226
6	2*	40	-77
7	2	61	79
8	2*	46	-5
9	2*	47	-19
10	2*	47	-33
11	2*	46	-9
12	2*	43	35
13	2*	35	11
0	3	75	64
1	3	197	195
2	3	145	-174
3	3	132	-139
4	3	214	213
5	3	39	34
6	3	59	-79
7	3*	44	-16
8	3*	46	-23
9	3*	47	24
10	3*	47	-7
11	3*	45	-12
12	3*	42	18
13	3*	32	7
0	4	33	-11
1	4*	34	14
2	4	163	198
3	4	36	-39
4	4	236	-252
5	4	41	24
6	4	137	131
7	4*	45	-50
8	4*	47	-52
9	4*	47	29
10	4	47	52
11	4*	44	-14
12	4	55	-44
0	5	383	-354
1	5	172	-164
2	5	252	232
3	5	161	164
4	5	129	-132
5	5	74	-75
6	5	149	158
7	5*	47	37
8	5	116	-111
9	5*	47	-20
10	5	46	22
11	5*	43	-9
12	5*	35	-5
0	6	88	75
1	6	80	-84
2	6	122	-135
3	6*	42	9
4	6	107	96
5	6*	45	18
6	6	66	-62
7	6*	47	-19
8	6*	47	41
9	6*	46	5
10	6*	44	-25
11	6*	39	-12
0	7*	43	17
1	7	61	61
2	7*	44	-5
3	7	110	-117
4	7*	46	16
5	7	124	130
6	7*	47	8
7	7*	47	-49
8	7*	46	-23
9	7*	45	19
10	7*	41	13
11	7	33	-31
0	8	205	-179
1	8	160	171
2	8	93	76
3	8	115	-109
4	8*	47	7

(*International Tables for X-ray Crystallography*, vol. 1, 1952), with approximate parameters 0·245, 0·81, 0·485 and 0·26, 0·09, 0·79. The geometric parts of the structure factor contributions of these sulfur atoms were calculated for the 659 observed reflections. Of these, 248 were greater than 0·6 in magnitude (the maximum

Table 1 (*cont.*)

H	K	FO	FC
5	8	82	69
6	8*	47	30
7	8	65	-42
8	8	45	-41
9	8*	41	18
10	8*	34	3
0	9	47	-35
1	9*	47	11
2	9	47	33
3	9*	47	24
4	9*	47	-8
5	9	47	-5
6	9	46	5
7	9*	44	12
8	9*	41	-25
9	9*	34	-23
0	10	66	-41
1	10	94	102
2	10	47	50
3	10	92	-112
4	10*	45	-37
5	10	63	65
6	10*	42	17
7	10*	38	-29
8	10*	32	-12
0	11	63	46
1	11	45	-16
2	11	44	-57
3	11*	43	67
4	11*	42	28
5	11*	38	-36
6	11*	34	-2
0	12	39	36
1	12	54	-76
2	12*	37	-21
3	12	35	43
4	12*	31	21
	L=	6	
0	0	148	140
1	0	466	459
2	0	184	-205
3	0	443	-447
4	0	233	196
5	0	237	235
6	0	72	-62
7	0	117	-101
8	0*	46	-28
9	0	47	-52
10	0*	47	-22
11	0*	45	-14
12	0	41	52
13	0*	32	7
0	1	31	-10
1	1	54	80
2	1	97	115
3	1	48	74
4	1	81	-97
5	1	67	-78
6	1*	42	17
7	1*	44	22
8	1	46	-5
9	1*	47	-29
10	1*	47	10
11	1*	45	51
12	1*	41	0
13	1	31	-25
0	2	45	24
1	2	152	-164
2	2	153	165
3	2	149	158
4	2	178	-202
5	2	69	-91
6	2	120	141
7	2*	45	55
8	2*	47	-77
9	2*	47	-43
10	2	47	33
11	2*	45	47
12	2*	40	-9
13	2*	29	-22
0	3	177	158
1	3	132	-126
2	3	268	-324
3	3	144	162
4	3	257	269
5	3	109	-140
6	3	123	-115
7	3	46	40
8	3*	47	56
9	3*	47	-13
10	3*	46	-49
11	3*	44	18
12	3*	38	27
0	4	291	256
1	4	109	-123
2	4	37	-49
3	4	78	55
4	4	100	-116
5	4*	43	-6
6	4	45	47
7	4*	47	-26
8	4*	47	0
9	4	47	6
10	4*	46	8
11	4*	43	10
12	4*	35	-3
0	5	39	-4
1	5	96	-98
2	5	120	-163
3	5	72	71
4	5	219	216
5	5	63	-58
6	5	66	-63
7	5*	47	33
8	5*	47	13
9	5	46	-9
10	5*	44	-30
11	5*	39	4
12	5	30	26
0	6	83	75
1	6	188	-149
2	6	74	-82
3	6	146	126
4	6	45	54
5	6	80	-73
6	6*	47	4
7	6*	47	14
8	6	47	-29
9	6*	45	-5
10	6*	42	8
11	6*	35	-2
0	7	256	-264
1	7*	45	32
2	7	137	221
3	7	46	-29
4	7	115	-107
5	7*	47	27
6	7	47	52
7	7	47	-46
8	7*	45	-52
9	7	43	24
10	7*	37	23
0	8*	47	-4
1	8	66	-79
2	8*	47	18
3	8	116	123
4	8*	47	-48
5	8	115	-98
6	8	46	24
7	8	45	19
8	8*	43	-4
9	8*	38	-1
10	8*	29	-1
0	9	47	-47
1	9	47	-73
2	9*	47	-32
3	9	81	58
4	9	66	60
5	9*	46	-21
6	9*	44	-19
7	9*	42	-14
8	9*	37	2
9	9*	29	14
0	10	93	86
1	10	167	150
2	10*	46	-39
3	10	120	-110
4	10*	44	-4
5	10	43	72
6	10*	39	-21
7	10	59	-56
0	11	97	-84
1	11*	43	42
2	11*	43	49
3	11*	41	-42
4	11*	38	-30
5	11	49	41
6	11	29	37
0	12*	35	-15
1	12	35	37
2	12*	33	6
3	12*	30	-9
	L=	7	
0	1	83	-80
1	1	109	-128
2	1	159	151
3	1	64	-105
4	1	192	-183
5	1	110	157
6	1	108	86
7	1	65	-68
8	1*	47	-20
9	1*	47	21
10	1*	46	9
11	1*	43	-5
12	1*	37	-5
0	2	121	94
1	2	138	125
2	2	82	-70
3	2	38	-63
4	2*	40	33
5	2	42	55
6	2*	45	-26
7	2*	46	-35
8	2*	47	33
9	2	47	11
10	2	46	-4
11	2*	43	16
12	2*	35	-14
0	3	73	76
1	3*	37	54
2	3	120	-134
3	3	304	-351
4	3	72	67
5	3	239	263
6	3*	46	3
7	3	47	-60
8	3*	47	-9
9	3*	47	35
10	3*	45	11
11	3*	42	-56
12	3*	33	-6
0	4	244	-236
1	4	214	228
2	4	166	196
3	4	156	-162
4	4	43	-45
5	4	101	115
6	4*	46	19
7	4	82	-69
8	4*	47	-40
9	4	46	15
10	4*	44	24
11	4*	39	12
0	5	124	114
1	5	276	-289
2	5	43	-45
3	5	236	208
4	5*	45	-15
5	5	114	-122
6	5*	47	-14
7	5	106	101
8	5*	47	31
9	5	78	-67
10	5*	42	-9
11	5*	35	31
0	6*	44	-2
1	6	99	-78
2	6*	45	-58
3	6	112	68
4	6	81	104
5	6*	47	-35
6	6*	47	-36
7	6*	47	-3
8	6*	46	-4
9	6	43	14
10	6*	38	0
0	7	146	143
1	7*	46	16
2	7	81	-108
3	7*	47	-10
4	7*	47	9
5	7*	47	4
6	7	47	-13
7	7	46	-10
8	7	44	37
9	7*	40	4
10	7*	32	-16
0	8	82	-82
1	8	82	-90
2	8	106	104
3	8	67	70
4	8	66	-95
5	8*	46	-25
6	8	64	51
7	8*	44	-7
8	8*	40	-24
9	8*	33	6
0	9	47	-46
1	9	66	-24
2	9	47	-8
3	9*	46	-6
4	9*	46	-7
5	9*	44	-8
6	9*	43	26
7	9*	38	20
8	9*	32	2
0	10	64	-41
1	10	45	-76
2	10	45	49
3	10	44	42
4	10*	42	-24
5	10*	39	7
6	10*	35	1
0	11	83	-86
1	11*	41	-9
2	11	55	74
3	11*	37	2
4	11	34	-55
5	11*	29	-9
0	12*	31	30
1	12*	30	-5
	L=	8	
0	0	139	-147
1	0	38	-70
2	0	86	78
3	0*	40	-22
4	0	60	-59
5	0	62	62
6	0	65	50
7	0*	47	-16
8	0	47	-38
9	0*	47	3
10	0*	45	22
11	0*	40	-14
12	0*	31	-9
0	1	314	-284
1	1	165	163
2	1	243	249
3	1	266	-270
4	1	134	-125
5	1	153	160
6	1	65	65
7	1*	47	-46
8	1	47	-57
9	1*	47	24
10	1	63	37
11	1*	40	-34
12	1*	30	-18
0	2	127	-121
1	2	219	-254
2	2	56	42
3	2	207	211
4	2	43	65
5	2	100	-76
6	2*	46	-56
7	2*	47	41
8	2*	47	18
9	2	65	-50
10	2*	44	-30
11	2*	39	20
0	3*	40	-34
1	3	40	43
2	3*	41	31
3	3	121	-116
4	3	44	46
5	3	65	76
6	3*	47	-53
7	3*	47	-22
8	3	47	16
9	3*	46	20
10	3*	43	2
11	3*	36	-16
0	4	83	-76
1	4	119	132
2	4*	43	-3
3	4	88	-85
4	4	64	86
5	4	47	70
6	4*	47	-26
7	4*	47	-33
8	4	47	-17
9	4*	45	5
10	4*	41	-6
11	4*	33	-5
0	5	44	46
1	5	63	65
2	5*	45	2
3	5	46	-25
4	5	47	13
5	5*	47	24
6	5*	47	-51
7	5*	47	-47
8	5	46	32
9	5*	43	32
10	5*	38	-14
0	6	46	15
1	6	179	182
2	6	66	-70
3	6	156	-139
4	6	67	70
5	6	67	66
6	6*	47	-24
7	6	46	-13
8	6*	44	10
9	6*	40	2
10	6*	32	-10
0	7*	47	0
1	7*	47	-22
2	7*	47	18
3	7*	47	-33
4	7*	47	2
5	7	66	9
6	7	46	-10
7	7*	44	31
8	7*	41	-4
9	7*	34	-20
0	8	67	-51
1	8*	47	-50
2	8	67	55
3	8	66	58
4	8	46	-16
5	8*	45	-15
6	8*	44	11
7	8*	40	7
8	8*	34	-5
0	9	153	140
1	9	46	-62
2	9	112	-119
3	9*	45	28
4	9	116	107
5	9*	42	-21
6	9	77	-77
7	9*	33	27
0	10*	44	-12
1	10*	43	42
2	10*	43	1
3	10*	41	-39
4	10	38	17
5	10*	34	34
0	11	37	-26
1	11*	36	-9
2	11	34	41
3	11*	31	20
	L=	9	
0	1	71	72
1	1	72	-38
2	1*	42	42
3	1	98	133
4	1*	45	-28
5	1	104	-107
6	1*	47	-26
7	1*	47	46
8	1*	47	10
9	1*	45	-24
10	1*	42	17
11	1*	34	18
0	2	59	29
1	2	112	-113
2	2*	43	-53
3	2	99	100
4	2	46	59
5	2*	47	-45
6	2*	47	-14
7	2*	47	4
8	2*	46	-2
9	2*	45	14
10	2*	41	-18
11	2*	32	-10
0	3	61	50
1	3	253	241
2	3*	44	-8
3	3*	45	-9
4	3*	46	-23
5	3*	47	-24
6	3*	47	-11
7	3	47	-59
8	3*	46	11
9	3	62	44
10	3*	39	4
11	3*	29	8
0	4	209	-208
1	4	78	-80
2	4	209	205
3	4	46	5
4	4	169	-176
5	4*	47	-54
6	4	105	99
7	4	47	72
8	4	45	-52
9	4*	42	-25
10	4*	36	29
0	5	65	-89
1	5	80	47
2	5	81	95
3	5*	47	23
4	5	47	-46
5	5*	47	-16
6	5*	47	-3
7	5*	46	-25
8	5*	44	12
9	5*	39	8
10	5*	31	-3
0	6	149	143
1	6*	47	-31
2	6	106	-115
3	6*	47	11
4	6*	47	66
5	6*	47	-18
6	6	46	-45
7	6*	44	28
8	6*	41	29
9	6*	34	-15
0	7	47	-55
1	7	157	151
2	7*	47	52
3	7	105	-129
4	7*	46	-8
5	7	45	70
6	7*	44	-4
7	7*	41	-41
8	7*	35	-11
0	8	47	23
1	8	81	81
2	8*	46	-14
3	8*	46	-32
4	8*	45	8
5	8*	43	5
6	8*	40	7
7	8*	35	3
0	9	63	39
1	9*	45	9
2	9*	44	-28
3	9	43	25
4	9*	41	34
5	9*	37	-32
6	9*	32	-31
0	10*	41	16
1	10*	40	46
2	10*	38	-23
3	10	36	-32
4	10*	32	7
0	11	31	30
1	11	51	-65
	L=	10	
0	0	224	198
1	0	288	274
2	0	111	-186
3	0	130	-138
4	0	94	95
5	0	47	36
6	0*	47	-40
7	0	47	-28
8	0*	45	30
9	0*	43	30
10	0*	36	-11
0	1	44	-73
1	1	77	-61
2	1	91	84
3	1	80	96
4	1	81	-90
5	1	95	-86
6	1*	47	54
7	1	81	43
8	1*	45	-28
9	1*	42	-16
10	1*	36	17
0	2	118	102
1	2*	45	-24
2	2*	46	-24
3	2*	47	18
4	2*	47	-22
5	2	47	-51
6	2*	47	-31
7	2	80	53
8	2*	45	53
9	2*	42	-16
10	2*	34	-7
0	3	194	193
1	3	80	-80
2	3	147	-136
3	3	47	75
4	3*	47	42
5	3*	47	-28
6	3*	47	-14
7	3*	46	8
8	3*	44	21
9	3*	40	-5
10	3*	32	-19
0	4	47	25
1	4	81	-52
2	4*	47	27
3	4*	47	-0
4	4	47	-62
5	4*	47	-22
6	4*	46	-7
7	4*	45	36
8	4*	43	35
9	4*	37	-13
0	5	47	36
1	5*	47	-61
2	5*	47	7
3	5*	47	14
4	5*	47	-42
5	5	47	14
6	5	79	44
7	5*	44	14
8	5*	39	-19
9	5*	32	-15
0	6	47	-60
1	6*	47	26
2	6*	47	41
3	6*	47	-15
4	6*	46	-32
5	6*	45	15
6	6	44	26
7	6*	41	-26
8	6*	35	-12
0	7	47	-30
1	7	81	77
2	7*	46	32
3	7	46	-63
4	7*	45	-44
5	7	43	30
6	7*	40	22
7	7*	35	-13
0	8*	45	-19
1	8	90	-88
2	8	44	11
3	8*	43	53
4	8*	42	-6
5	8	38	-50
6	8*	34	-7
0	9	73	70
1	9	42	54
2	9	57	-59
3	9	38	-33
4	9*	35	14
5	9	30	33
0	10*	35	13
1	10*	34	53
2	10*	31	-12
	L=	11	
0	1*	47	-27
1	1	47	54
2	1*	47	-19
3	1*	47	-25
4	1	47	21
5	1*	47	3
6	1*	46	4
7	1*	45	4
8	1*	42	-5
9	1*	36	-2
0	2	175	189
1	2*	47	-24
2	2	82	-103
3	2	47	-12
4	2*	47	41
5	2*	47	21
6	2*	46	-50
7	2*	44	9
8	2	41	43
9	2*	35	-18
0	3	67	-65
1	3	47	44
2	3*	47	9
3	3	47	-54
4	3*	47	-4
5	3	47	35
6	3*	45	56
7	3*	44	5
8	3*	39	-44
9	3	32	-6
0	4*	47	-16
1	4*	47	10
2	4*	47	4
3	4*	47	5
4	4*	47	-2
5	4*	46	-11
6	4*	44	14
7	4*	42	13
8	4*	36	-21
0	5	47	13
1	5	188	-172
2	5*	47	-3
3	5	123	121
4	5*	46	20
5	5	100	-83
6	5*	43	-6
7	5*	39	63
8	5*	32	-6
0	6	66	62
1	6*	46	-8
2	6	46	-58
3	6*	45	-3
4	6	77	37
5	6*	43	18
6	6*	39	-17
7	6*	34	-14
0	7	45	13
1	7*	45	-12
2	7*	44	-13
3	7*	43	13
4	7*	42	5
5	7*	38	-5
6	7*	33	8
0	8	43	-54
1	8	95	-75
2	8	82	60
3	8*	39	28
4	8	71	-53
5	8*	31	-8
0	9	37	-22
1	9*	35	-14
2	9*	33	4
3	9*	30	7
	L=	12	
0	0	82	-65
1	0*	47	46
2	0	47	68
3	0	47	-47
4	0	81	-69
5	0	65	64
6	0	44	39
7	0*	42	-59
8	0*	36	-7
0	1	125	-109
1	1*	47	22
2	1*	47	47
3	1*	47	-22
4	1	47	-16
5	1*	46	-2
6	1*	44	24
7	1*	41	16
8	1*	35	-21
0	2*	47	-18
1	2*	47	-58
2	2*	47	9
3	2	47	60
4	2*	46	12
5	2*	45	-27
6	2*	44	0
7	2*	40	-9
8	2*	34	-13
0	3*	47	-9
1	3	94	102
2	3*	47	-16
3	3	93	-80
4	3*	46	27
5	3	45	55
6	3*	43	-13
7	3*	38	-33
8	3*	31	-1
0	4	47	25
1	4	47	67
2	4*	46	-32
3	4*	46	-20
4	4	45	31
5	4*	43	14
6	4*	40	4
7	4*	35	-32
0	5	46	28
1	5*	46	49
2	5*	45	-21
3	5*	45	-19
4	5*	43	17
5	5*	41	13
6	5*	36	-24
7	5*	30	-22
0	6	63	75
1	6*	44	-6
2	6*	44	-43
3	6	43	16
4	6*	40	7
5	6	36	-8
6	6*	31	0
0	7	127	-91
1	7*	42	-29
2	7	57	55
3	7*	38	31
4	7*	35	-35
5	7*	29	-24
0	8	37	27
1	8*	36	-34
2	8*	34	-4
3	8	43	27
	L=	13	
0	1	66	-41
1	1	147	-126
2	1*	46	29
3	1	45	56
4	1*	44	-12
5	1*	43	-31
6	1*	39	3
7	1*	33	27
0	2	46	-35
1	2	46	49
2	2*	46	17
3	2*	45	-21
4	2*	44	10
5	2*	42	19
6	2*	37	-8
7	2	31	-24
0	3	46	10
1	3*	46	26
2	3*	45	13
3	3*	44	-27
4	3*	43	-33
5	3*	40	33
6	3*	35	4
0	4	78	-78
1	4*	45	-14
2	4	76	45
3	4*	43	22
4	4*	41	-30
5	4*	37	-19
6	4*	32	10
0	5	44	33
1	5*	43	-21
2	5*	42	-38
3	5*	40	-0
4	5*	37	-28
5	5*	33	2
0	6	58	59
1	6*	40	17
2	6*	38	-38
3	6*	36	-4
4	6*	32	28
0	7*	35	-15
1	7	34	46
2	7*	32	4
	L=	14	
0	0	45	-47
1	0	44	40
2	0*	43	36
3	0*	42	-21
4	0*	39	-14
5	0*	35	17
6	0*	29	25
0	1	45	-44
1	1*	44	-26
2	1*	43	47
3	1*	42	33
4	1	39	-48
5	1*	35	-22
0	2*	44	18
1	2*	44	-26
2	2*	43	-31
3	2*	41	3
4	2	38	39
5	2*	33	-0
0	3*	43	1
1	3*	43	-38
2	3*	41	16
3	3*	39	30
4	3*	35	-16
5	3*	30	-20
0	4	41	-55
1	4*	40	-5
2	4*	38	32
3	4*	36	-17
4	4*	32	-14
0	5	38	-39
1	5*	36	-21
2	5*	34	34
3	5*	31	6
0	6	56	-54
1	6	31	35
	L=	15	
0	1	68	64
1	1	38	43
2	1*	36	-47
3	1*	33	-5
0	2	53	60
1	2*	36	-4
2	2*	34	-40
3	2*	31	-15
0	3	50	-18
1	3*	34	17
2	3*	32	18
0	4*	32	-13
1	4*	30	-20

possible was 2·0), and these terms were used in calculating a three-dimensional Fourier map. Only two of these 248 phases were eventually found to be incorrect.

In addition to confirming the sulfur atom positions this Fourier showed two of the carbon atoms and six of the boron atoms. A second three-dimensional Fourier was computed using the 448 terms for which the contributions of these atoms was largest. At this stage positions were obtained for all except the hydrogen atoms. The parameters were refined by the method of least squares, using the IBM 704 program of Busing & Levy (1959*a*). Individual isotropic temperature factors were assigned to all atoms and were included in the refinements. Ten scale factors were also refined, one for each value of l. The atomic scattering factors used were those of Viervoll & Øgrim (1949) for S, Berghuis *et al.* (1955) for C, Ibers (1957) for B, and McWeeny (1951) for H. Only the observed reflections were used. The final reliability factor, $R=\Sigma|F_o-F_c|/\Sigma F_o$, was 0·174.

The results of these refinements were used in the computation of a difference Fourier. Only four hydrogen atoms were unambiguously located by this calculation, and attempts to refine the positions of these atoms by the least squares method were unsuccessful. Furthermore, the boron–boron distances obtained at this stage of the analysis did not agree with those of $B_{10}H_{12}(CH_3CN)_2$ (Reddy & Lipscomb, 1959), nor were they consistent with the C_{2v} molecular symmetry of decaborane (Kasper, Lucht & Harker, 1950). All subsequent work was, therefore, carried out using the counter data.

Only the 1828 observed reflections were used in most of the remaining work. After refining the S, C, and B positions and isotropic temperature factors with this improved data to a reliability factor of 0·20, another difference Fourier was computed. Approx-

Table 2. *Atomic parameters of* $B_{10}H_{12}[S(CH_3)_2]_2$

Atom	*x*	*y*	*z*	*B* (Å^2)
S1	0·2424 ± 0·0003	0·6965 ± 0·0002	0·9760 ± 0·0002	—
S2	0·2648 ± 0·0003	0·0874 ± 0·0003	0·7904 ± 0·0002	—
C1*A*	0·355 ± 0·001	0·673 ± 0·001	0·080 ± 0·001	—
C1*B*	0·111 ± 0·001	0·686 ± 0·001	0·043 ± 0·001	—
C2*A*	0·394 ± 0·001	0·047 ± 0·001	0·872 ± 0·001	—
C2*B*	0·157 ± 0·001	0·029 ± 0·001	0·872 ± 0·001	—
B1	0·303 ± 0·001	0·484 ± 0·001	0·687 ± 0·001	6·1 ± 0·3
B2	0·227 ± 0·001	0·577 ± 0·001	0·767 ± 0·001	5·4 ± 0·2
B3	0·150 ± 0·001	0·471 ± 0·001	0·687 ± 0·001	5·9 ± 0·3
B4	0·236 ± 0·001	0·337 ± 0·001	0·689 ± 0·001	4·8 ± 0·2
B5	0·358 ± 0·001	0·526 ± 0·001	0·814 ± 0·001	5·8 ± 0·3
B6	0·243 ± 0·001	0·541 ± 0·001	0·901 ± 0·001	4·7 ± 0·2
B7	0·109 ± 0·001	0·503 ± 0·001	0·816 ± 0·001	5·8 ± 0·3
B8	0·119 ± 0·001	0·339 ± 0·001	0·765 ± 0·001	5·9 ± 0·3
B9	0·255 ± 0·001	0·263 ± 0·001	0·812 ± 0·001	4·9 ± 0·2
B10	0·368 ± 0·001	0·360 ± 0·001	0·761 ± 0·001	5·7 ± 0·3
H1	0·31 ± 0·01	0·53 ± 0·01	0·60 ± 0·01	—
H2	0·22 ± 0·01	0·68 ± 0·01	0·76 ± 0·01	—
H3	0·11 ± 0·01	0·51 ± 0·01	0·60 ± 0·01	—
H4	0·23 ± 0·01	0·27 ± 0·01	0·63 ± 0·01	—
H5	0·44 ± 0·01	0·58 ± 0·01	0·83 ± 0·01	—
H6	0·25 ± 0·01	0·47 ± 0·01	0·96 ± 0·01	—
H7	0·02 ± 0·01	0·54 ± 0·01	0·83 ± 0·01	—
H8	0·03 ± 0·01	0·29 ± 0·01	0·75 ± 0·01	—
H9	0·26 ± 0·01	0·28 ± 0·01	0·90 ± 0·01	—
H10	0·45 ± 0·01	0·33 ± 0·01	0·75 ± 0·01	—
H7–8	0·11 ± 0·01	0·40 ± 0·01	0·84 ± 0·01	—
H5–10	0·37 ± 0·01	0·42 ± 0·01	0·84 ± 0·01	—

imate positions were obtained for the 12 decaborane hydrogen atoms, but the methyl group hydrogens were still not clearly established. The four largest peaks on this difference map consisted of two peaks near each of the sulfur atoms, suggesting anisotropic thermal motion. Anisotropic temperature factors were assigned to the S and C atoms and were refined along with the positions of these atoms (the B and H parameters were kept fixed in this treatment). The reliability factor after this calculation was 0·148; when the H atoms were omitted it was 0·153. The standard error of fit, $[\Sigma(F_o-F_c)^2/(m-n)]^{\frac{1}{2}}$, was 2·4. $m=1828$ was the number of observations, $n=95$ was the number parameters being adjusted. It has not proved possible to refine the parameters of the decaborane hydrogens, nor did a final difference Fourier locate the methyl hydrogens.

Table 1 compares the observed and calculated structure factors; the values listed have been multiplied by 10.

Table 2 lists the parameters of the atoms, including the isotropic temperature factors of the boron atoms. The standard errors listed were computed by Busing & Levy's least-squares program by the method given in the *International Tables for X-ray Crystallography*, vol. 2, pp. 330 (1959). The errors given for the hydrogen atom parameters, however, are estimates based on the assumption of *mm*2 molecular symmetry.

Transformation to Cartesian coordinates

For ease in visualizing and discussing this structure, the parameters have been transformed to a set of Cartesian axes aligned with the symmetry elements of the decaborane molecule. An orthogonal system was selected with axes normalized to 1*A* and **b**′ and **c**′ parallel to the monoclinic **b** and **c**, respectively. The molecule was rotated in this system of axes to make the average boron–boron vector given by

Table 3. *Atomic parameters of* $B_{10}H_{12}[S(CH_3)_2]_2$ *transformed to a 1A Cartesian system*

Atom	*x*′	*y*′	*z*′
S1	0·037	3·534	8·893
S2	−0·003	−3·457	9·083
C1*A*	1·22	3·68	10·26
C1*B*	−1·60	3·86	9·67
C2*A*	1·39	−3·59	10·25
C2*B*	−1·42	−3·57	10·23
B1	0·93	−0·02	6·33
B2	0·00	1·37	6·90
B3	−0·91	0·00	6·31
B4	0·01	−1·41	6·89
B5	1·49	0·95	7·73
B6	0·00	1·62	8·61
B7	−1·53	0·96	7·73
B8	−1·51	−0·94	7·73
B9	0·01	−1·59	8·65
B10	1·50	−0·95	7·72
H1	1·1	0·0	5·2
H2	−0·1	2·4	6·4
H3	−1·5	0·3	5·4
H4	−0·4	−2·3	6·3
H5	2·5	1·3	7·5
H6	0·4	1·2	9·6
H7	−2·6	1·6	7·6
H8	−2·6	−1·5	7·8
H9	0·1	−1·1	9·8
H10	2·6	−1·4	7·6
H7–8	−1·4	0·0	8·3
H5–10	1·7	0·0	8·5

Table 4. *Anisotropic temperature factors, before and after transformation to Cartesian axes*

		Component					
Atom	Tensor	11	22	33	12	13	23
S1	B	0·0152 ± 0·0004	0·0074 ± 0·0002	0·0082 ± 0·0002	0·0002 ± 0·0002	0·0020 ± 0·0002	−0·0005 ± 0·0002
	B′	2·07	0·86	1·31	0·01	0·19	0·09
S2	B	0·0190 ± 0·0004	0·0081 ± 0·0002	0·0080 ± 0·0002	0·0005 ± 0·0003	0·0033 ± 0·0002	−0·0006 ± 0·0002
	B′	2·58	0·91	1·33	0·07	0·37	0·03
C1*A*	B	0·0172 ± 0·0017	0·0130 ± 0·0014	0·0123 ± 0·0012	−0·0002 ± 0·0013	−0·0020 ± 0·0011	−0·0036 ± 0·0010
	B′	2·48	1·27	2·22	−0·23	−0·46	−0·17
C1*B*	B	0·0183 ± 0·0017	0·0230 ± 0·0020	0·0180 ± 0·0016	−0·0035 ± 0·0016	0·0101 ± 0·0014	−0·0083 ± 0·0015
	B′	2·25	1·92	3·72	0·13	1·19	−0·85
C2*A*	B	0·0138 ± 0·0014	0·0126 ± 0·0013	0·0166 ± 0·0015	0·0038 ± 0·0011	0·0025 ± 0·0012	0·0016 ± 0·0011
	B′	1·95	1·70	2·37	0·45	−0·02	0·59
C2*B*	B	0·0150 ± 0·0015	0·0128 ± 0·0012	0·0147 ± 0·0013	−0·0014 ± 0·0011	0·0017 ± 0·0011	0·0048 ± 0·0011
	B′	2·03	2·08	1·82	−0·23	0·19	0·76

B5–B7, B1–B3, B8–B10 parallel to **a**′ and the average of B5–B10, B7–B8, B2–B4, B6–B9, parallel to **b**′. (The S–S and C–C vectors deviated too much from the assumed symmetry to be included in the derivation of this transformation). Finally, the molecule was translated to place the molecular 2-fold axis coincident with **c**′. The resultant transformation, in terms of a matrix M and a vector **t**, was applied to the atomic coordinates, **x**, to give $\mathbf{x}' = M\mathbf{x} + \mathbf{t}$, where

$$M = \begin{pmatrix} 11{\cdot}792 & 0{\cdot}868 & -1{\cdot}209 \\ -0{\cdot}867 & 10{\cdot}018 & 4{\cdot}682 \\ 0{\cdot}402 & -3{\cdot}889 & 11{\cdot}787 \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} -2{\cdot}246 \\ -7{\cdot}803 \\ 0 \end{pmatrix}.$$

These transformed coordinates are listed in Table 3.

The transformation of the anisotropic temperature factors to the orthonormal system, derived from the invariance of the quadratic form $\Sigma\beta_{ij}h_ih_j$, is $B' = MBM^T$, where B is the anisotropic temperature factor tensor in terms of the original monoclinic axes,

Table 5. *Principal values and directions of anisotropic temperature factors*

Atom	Component	Principal value	Direction referred to Cartesian axes
S1	1	2·12	(0·973, 0·020, 0·228)
	2	0·85	(−0·026, −0·980, 0·196)
	3	1·29	(−0·228, 0·197, 0·954)
S2	1	2·69	(0·964, 0·044, 0·264)
	2	0·90	(0·034, −0·999, 0·040)
	3	1·22	(−0·265, 0·030, 0·964)
C1*A*	1	2·83	(−0·805, 0·054, 0·591)
	2	1·16	(0·256, 0·930, 0·263)
	3	1·98	(0·535, −0·364, 0·762)
C1*B*	1	2·18	(−0·674, −0·729, 0·120)
	2	1·14	(−0·600, 0·635, 0·486)
	3	4·56	(0·431, −0·256, 0·865)
C2*A*	1	2·09	(−0·845, −0·247, 0·474)
	2	1·15	(0·455, −0·798, 0·396)
	3	2·77	(0·280, 0·550, 0·786)
C2*B*	1	2·12	(0·950, −0·132, 0·282)
	2	2·72	(−0·080, 0·772, 0·631)
	3	1·09	(−0·301, −0·622, 0·723)

Table 6. *Comparison of bond lengths of* $B_{10}H_{12}[S(CH_3)_2]_2$, $B_{10}H_{12}(CH_3CN)_2$, and $B_{10}H_{14}$

	$B_{10}H_{12}[S(CH_3)_2]_2$	$B_{10}H_{12}(CH_3CN)_2$	$B_{10}H_{14}$
S1–C1*A*	1·81 ± 0·01 Å	—	—
–C1*B*	1·84 ± 0·02	—	—
–B6	1·93 ± 0·01	—	—
S2–C2*A*	1·82 ± 0·01	—	—
–C2*B*	1·83 ± 0·01	—	—
–B9	1·92 ± 0·01	—	—
B1–B2	1·76 ± 0·02	1·764 Å	1·80 Å
–B3	1·84 ± 0·02	1·837	1·71
–B4	1·76 ± 0·02	1·749	1·78
–B5	1·80 ± 0·02	1·790	1·77
–B10	1·77 ± 0·02	1·766	1·78
–H1	1·17	1·18	1·16
B2–B3	1·74 ± 0·02	1·749	1·78
–B5	1·76 ± 0·02	1·742	1·80
–B6	1·74 ± 0·02	1·746	1·72
–B7	1·78 ± 0·02	1·746	1·76
–H2	1·12	1·10	1·27
B3–B4	1·78 ± 0·02	1·764	1·80
–B7	1·81 ± 0·02	1·766	1·78
–B8	1·80 ± 0·02	1·790	1·77
–H3	1·35	1·18	1·16
B4–B8	1·79 ± 0·02	1·742	1·80
–B9	1·76 ± 0·02	1·746	1·72
–B10	1·77 ± 0·02	1·746	1·76
–H4	1·19	1·10	1·27
B5–B6	1·87 ± 0·02	1·860	1·77
–B10	1·91 ± 0·02	1·881	2·01
–H5	0·91	1·11	1·22
–H5–10	1·23	1·23	—
B6–B7	1·88 ± 0·02	1·849	1·77
–H6	1·13	1·C6	1·28
B7–B8	1·91 ± 0·02	1·881	2·01
–H7	1·27	1·06	1·35
–H7–8	1·22	1·22	—
B8–B9	1·88 ± 0·02	1·860	1·77
–H8	1·25	1·11	1·22
–H7–8	1·02	1·23	—
B9–B10	1·87 ± 0·02	1·849	1·77
–H9	1·25	1·06	1·28
B10–H10	1·17	1·06	1·35
–H5–10	1·31	1·22	—

B' is the transformed tensor, and M^T is the transpose of matrix M. The principal axes of the thermal vibration ellipsoids are obtained from the characteristic equations of the B' tensors. These calculations have been checked by Waser's method (1955) by which the principal axes were found in terms of the monoclinic axes; the reciprocal lattice directions obtained were converted to our Cartesian system by the matrix $(M^{-1})^T$. Both the original and the transformed components of the thermal vibration tensors of the S and C atoms are listed in Table 4. The principal values and directions of the principal axes, referred to the Cartesian coordinate system, are given in Table 5.

Discussion

Table 6 lists the interatomic distances of the $B_{10}H_{12}[S(CH_3)_2]_2$ molecule. The corresponding distances of $B_{10}H_{12}(CH_3CN)_2$ (Reddy & Lipscomb, 1959) and of $B_{10}H_{14}$ (Moore, Dickerson & Lipscomb, 1957) are included for comparison. The distances and standard errors of $B_{10}H_{12}[S(CH_3)_2]_2$ were computed by Busing & Levy's IBM 704 Function and Error Program (1959*b*). The standard deviations of the $B_{10}H_{12}(CH_3CN)_2$ distances are 0·008 for B–B and 0·04 for B–H; in the case of $B_{10}H_{14}$ the standard deviations are 0·016 for B–B and 0·09 for B–H.

The $B_{10}H_{12}[S(CH_3)_2]_2$ distances other than those

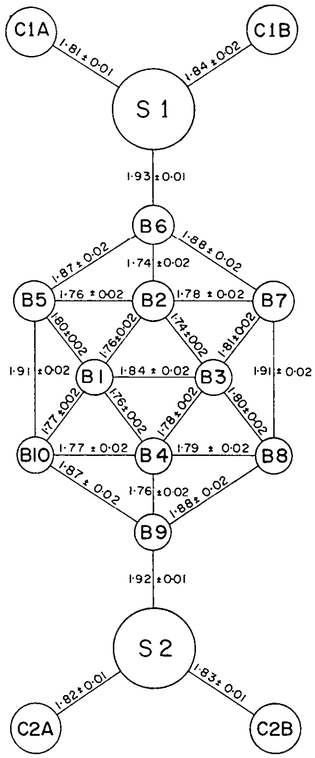

Fig. 1. Bond lengths of $B_{10}H_{12}[S(CH_3)_2]_2$.

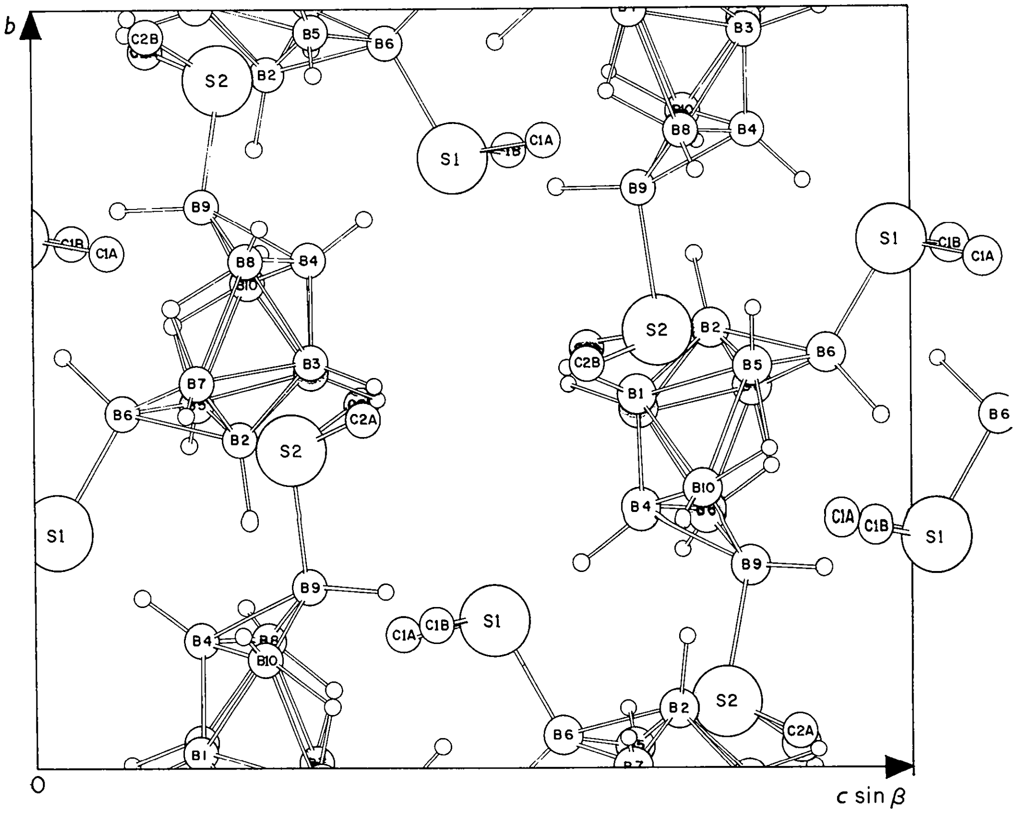

Fig. 2. Molecular packing in $B_{10}H_{12}[S(CH_3)_2]_2$.

involving hydrogen are shown in Fig. 1; bond lengths related by the molecular symmetry are seen to agree closely.

The C–S–C bond angles (104·2 ± 1·4° and 100·6 ± 1·3°) and S–C bond lengths are within experimental error of the angle of about 105° and distance of 1·82 Å reported for $(CH_3)_2S$ by Brockway & Jenkins (1936). The S–B bond lengths are what would be expected for a normal covalent bond.

The decaborane structure has four hydrogens bridging the pairs B5–B6, B6–B7, B8–B9, B9–B10; both $B_{10}H_{12}[S(CH_3)_2]_2$ and $B_{10}H_{12}(CH_3CN)_2$ have just the two bridges B5–B10 and B7–B8. Although the corresponding distances in the two derivatives are very similar, they differ significantly from the distances in decaborane. However, the average of the 21 B–B bond lengths is 1·809 Å for $B_{10}H_{12}[S(CH_3)_2]_2$ and 1·792 Å for both $B_{10}H_{12}(CH_3CN)_2$ and $B_{10}H_{14}$. The average length of our 10 terminal B–H bonds is 1·18 Å, which is 0·08 Å greater than the corresponding average for $B_{10}H_{12}(CH_3CN)_2$ and 0·08 Å less than for decaborane.

Table 3 demonstrates the C_{2v} symmetry of the decaborane skeleton. The deviations of the $(CH_3)_2S$ groups from this symmetry may perhaps be attributed to steric effects. Reddy & Lipscomb (1959) have discussed the valence structure of $B_{10}H_{12}(CH_3CN)_2$ in terms of the topological theory of boron hydrides (Dickerson & Lipscomb, 1957). The structure is compatible with this representation if it is regarded as a substitution derivative of the $B_{10}H_{14}^{-2}$ ion, which has C_{2v} symmetry. Reddy & Lipscomb have suggested a possible mechanism for the reaction of an electron donor with this ion.

The arrangement of $B_{10}H_{12}[S(CH_3)_2]_2$ molecules in the monoclinic unit cell is shown in Fig. 2.

We wish to thank Dr M. F. Hawthorne of the Rohm & Haas Company for supplying us with samples of $B_{10}H_{12}[S(CH_3)_2]_2$. We also thank Dr Howard C. Hornig for his interest in this problem and for several valuable discussions. Finally, we express our appreciation to Mrs Iven M. Moen for assistance in the measurement of the spectrometric intensities.

References

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Brockway, L. O. & Jenkins, H. O. (1936). *J. Amer. Chem. Soc.* **58**, 2036.

Busing, W. R. & Levy, H. A. (1959*a*). *A Crystallographic Least Squares Refinement Program for the* IBM 704. Oak Ridge National Laboratory Report 59-4-37.

Busing, W. R. & Levy, H. A. (1959*b*). *A Crystallographic Function and Error Program for the* IBM 704. Oak Ridge National Laboratory Report 59-12-3.

Dickerson, R. E. & Lipscomb, W. N. (1957). *J. Chem. Phys.* **27**, 212.

Ibers, J. A. (1957). *Acta Cryst.* **10**, 86.

International Tables for X-ray Crystallography (1952). Vol. 1. Birmingham: Kynoch Press.

International Tables for X-ray Crystallography (1959). Vol. 2. Birmingham: Kynoch Press.

Kasper, J. S., Lucht, C. M. & Harker, D. (1950). *Acta Cryst.* **3**, 436.

McWeeny, R. (1951). *Acta Cryst.* **4**, 513.

Moore, E. B., Jr., Dickerson, R. E. & Lipscomb, W. N. (1957). *J. Chem. Phys.* **27**, 209.

Reddy, J. van der Maas and Lipscomb, W. N. (1959). *J. Chem. Phys.* **31**, 610.

Tulinsky, A., Worthington, C. R. & Pignataro, E. (1959). *Acta Cryst.* **12**, 623.

Viervoll, H. & Øgrim, O. (1949). *Acta Cryst.* **2**, 277.

Waser, J. (1955). *Acta Cryst.* **8**, 731.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1962). **15**, 417

Atomic scattering amplitudes for electrons for some of the lighter elements.

By B. Dawson,
Division of Chemical Physics, C.S.I.R.O. Chemical Research Laboratories, Melbourne, Australia

(*Received* 2 *November* 1961)

New values of atomic scattering amplitudes, $f_{el}(s)$ ($s = \sin\theta/\lambda$), in the first Born approximation, have recently been derived for the neutral atoms Al to A inclusive by a process of interpolation (Dawson, 1961*a*). The interpolation procedure was concerned primarily with the derivation of values of the mean square radii $\langle r^2\rangle$ of the atomic charge distributions, and it was observed that the main uncertainty in this procedure lay in values of $\langle r^2\rangle_{3p}$ derived from curve *C* (Fig. 1 and Table 1(*B*) of Dawson, 1961*a*). To minimize this uncertainty, the upper (i.e. higher atomic number, *Z*) end of this curve was adjusted to give interpolated total $\langle r^2\rangle$ values for Cl and A in best agreement with the polydetor $\langle r^2\rangle$ result for Cl and the experimental $\langle r^2\rangle$ value for argon. A more critical appraisal of various aspects of the interpolation process is now possible in view of recent Hartree–Fock calculations by Watson & Freeman (1961) for these neutral atoms and by Sachs (1961) for