Table 6. *Comparison of trihalide ions*

Compound	Ion	Bond lengths (Å)		Elongation* (Å)		Sum (Å)
See footnote†	I–I–I	2·92	2·92	0·26	0·26	0·52
CsI_3	I–I–I	2·83	3·03	0·17	0·37	0·54
CsI_2Br	I–I–Br	2·78	2·91	0·12	0·43	0·55
NH_4BrICl	Br–I–Cl	2·51	2·91	0·03	0·59	0·62‡

* Relative to the bond lengths of gaseous molecules I_2, IBr and ICl.

† Average values from $As(C_6H_5)_4I_3$, $N(C_2H_5)_4I_7$ and $N(C_2H_5)_4I_3$ (Rundle, 1961; Migchelsen & Vos, 1967).

‡ Values are approximate because of disorder.

that of chlorine. The bond lengths listed for ion *A* in Fig. 3(*a*) are compared with those of other trihalide ions in Table 6. The $(BrICl)^-$ ion in NH_4BrICl fits well in the series. The present results suggest that the I–Cl bond in NH_4BrICl (*A*) has a smaller bond order than the I–Br bond in the isomorphous compound CsI_2Br (Carpenter, 1966).

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The Crystal Structure of Sodium Tetraborate

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Single crystals of the high-temperature form of sodium tetraborate, $Na_2O.4B_2O_3$, have been synthesized and studied. The structure has been determined by the method of symbolic addition. The space group is $P2_1/a$ with unit-cell dimensions $a = 6{\cdot}507 \pm 0{\cdot}001$,† $b = 17{\cdot}796 \pm 0{\cdot}002$, $c = 8{\cdot}377 \pm 0{\cdot}001$ Å; $\beta = 96°34' \pm 2'$; $Z = 4$. The structure consists of two infinite, independent, and interlinking boron–oxygen networks, each containing alternating single and double rings. The sodium atoms serve to hold the networks together through coordination with oxygen atoms.

Introduction

This study has been made as part of a program designed for a better understanding of the structural principles underlying borate chemistry. There is additional interest in anhydrous borates with greater than 50 mole % B_2O_3 since these compounds readily form glasses. Several laboratories have been investigating these structures. Krogh-Moe (1959, 1960, 1962, 1965) has reported structures of anhydrous borates of K and Rb, Cs, Li, and Ag. The structures of strontium 1:2 borate (Krogh-Moe, 1964; Perloff & Block, 1966), lead 1:2 borate (Perloff & Block, 1966), barium 1:2 borate (Block & Perloff, 1965) and cadmium 1:2 borate (Ihara & Krogh-Moe, 1966) have also been determined. The structure of $Na_2O.4B_2O_3$ and its relation to several other borates are discussed here.

$Na_2O.4B_2O_3$ has been reported (Morey & Merwin, 1936) to exist in two forms. The present work refers to the high-temperature stable form which is usually obtained by crystallization from a melt.

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† Estimated uncertainty.

Experimental

Single crystals of sodium 1:4 borate were grown from a stoichiometric melt on a hot wire loop. Precession photographs showed systematic extinctions occurring only in the $h0l$ ($h=2n+1$) and $0k0$ ($k=2n+1$) reflections. This confirmed Krogh-Moe's (1965) space group determination as $P2_1/a$. Intensity data were collected with the aid of a General Electric single-crystal orienter and diffractometer, used in conjunction with a scintillation counter, and pulse height analyzer. Using Cu $K\alpha$ radiation ($\lambda=1·54051$ Å), the positions of high angle reflections were observed, yielding the following unit cell parameters:*

$a=6·507\pm0·001$ Å
$b=17·796\pm0·002$
$c=8·377\pm0·001$
$\beta=96°34'\pm2'$

$Z=4$ (derived from density of 2·32 g.cm^{-3} measured by Krogh-Moe, 1957).

Mo $K\alpha$ radiation ($\lambda=0·710688$ Å) was used to collect intensity data. For each reflection, fixed time (10 s) measurements were made of the peak height and background intensities. The peak heights were later converted to integrated intensities by preparing an empirical calibration curve of the ratio of peak height to integrated intensity as a function of the scattering angle.

Structure determination

Because of the small size of the particular crystal studied no absorption corrections were deemed necessary ($0·01<\mu R<0·015$). The set of intensities were corrected by the appropriate Lorentz and polarization factors, and reduced to scaled values of normalized structure factors, *i.e.* E_{hkl} (Hauptman & Karle, 1953).

The symbolic addition method of Karle & Karle (1963) was used to assign phases to the E_{hkl}. The quantities E_{214}, E_{175} and E_{172} were arbitrarily chosen as positive. This fixed the origin and provided a starting point for the generation of more signs *via* Hauptman & Karle's (1953) Σ_2 relation. (*i.e.* $sE_{\mathbf{h}}=s\,\Sigma_{\mathbf{k}}E_{\mathbf{k}}E_{\mathbf{h}-\mathbf{k}}$ in which s is read *sign of*). Using the formula

$$P_{\pm}(E_{\mathbf{h}})=\tfrac{1}{2}\pm\tfrac{1}{2}\tanh\,[\sigma_3/\sigma_2^{3/2}\,\Sigma\,|E_{\mathbf{h}}|E_{\mathbf{h}-\mathbf{k}}E_{\mathbf{k}}]\,,$$

twenty-two of the first twenty-three signs generated had probabilities greater than 0·95 of being correct, the remaining phase being assigned with an associated probability of 0·90. Thereafter a criterion was established such that no new sign was accepted as 'known' unless it had an associated probability of being correct $\geq 0·989$. When during the course of this sign generating procedure a probability fell below this level, the corresponding phase was deleted from the 'known' list. In this way the list of phases was built up, without using any letters, to include 181 of the 209 E_{hkl} with magnitudes $\geq 1·8$.

This procedure, however, led to a false set of signs. This was revealed by an E map which contained too many peaks, not the expected distribution of peak magnitudes, and no chemically sensible structure could be derived from the map. An examination of the mechanism through which the signs were being generated revealed that E_{200} entered into more contributing pairs *via* Σ_2 than any other reflection. In addition, E_{200} had been assigned a negative value very early in the procedure. An application of the Σ_1 relation of Karle & Hauptman to this reflection gave an indication that the sign is positive. The original assignment of E_{200} as negative was traced back through several steps to

Table 1. *Atomic parameters*

	x	$\sigma_x\times10^5$	y	$\sigma_y\times10^5$	z	$\sigma_z\times10^5$	B	$\sigma_B\times10^3$
Na(1)	0·40913	32	0·36344	12	0·02913	25	1·492	35
Na(2)	0·04214	32	0·40039	11	0·57361	25	1·396	35
O(1)	0·28617	48	0·56295	18	0·85698	37	0·870	46
O(2)	0·62003	51	0·53402	18	0·81618	39	0·994	48
O(3)	0·95484	47	0·52147	18	0·72816	37	0·791	45
O(4)	0·71036	48	0·42652	18	0·67233	37	0·862	46
O(5)	0·36111	49	0·44174	18	0·74677	37	0·901	46
O(6)	0·41744	49	0·36845	18	0·52297	39	0·915	47
O(7)	0·51672	50	0·24090	18	0·57164	39	1·008	48
O(8)	0·54274	47	0·18998	18	0·82597	37	0·794	45
O(9)	0·53633	48	0·32488	18	0·79325	37	0·835	46
O(10)	0·39526	53	0·28356	19	0·30888	40	1·131	50
O(11)	0·40497	49	0·22939	18	0·06349	38	0·904	46
O(12)	0·51686	48	0·10347	17	0·03420	37	0·812	46
O(13)	0·43583	47	0·14858	17	0·29426	36	0·808	46
B(1)	0·41418	71	0·51139	26	0·80289	54	0·771	62
B(2)	0·76351	73	0·49430	27	0·74188	56	0·870	63
B(3)	0·51060	69	0·39208	26	0·68252	53	0·676	59
B(4)	0·44396	73	0·29906	27	0·46961	57	0·888	64
B(5)	0·53140	69	0·25489	25	0·73447	54	0·691	60
B(6)	0·41239	71	0·21720	26	0·22871	54	0·745	60
B(7)	0·48233	70	0·17267	25	0·97369	54	0·739	61
B(8)	0·43147	66	0·08211	25	0·18553	52	0·588	57

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* The uncertainties quoted on all the cell dimensions are estimates based on past experience with the experimental apparatus. In the authors' opinion a conservative estimate of error will be obtained if these uncertainties are treated as standard deviations.

Table 2. *Final observed and calculated structure factors*

The columns are l, $10sF_o$ and $10F_c$, respectively with $s = 1{\cdot}0526$. Unobserved reflections are indicated with * and have been given F_o values corresponding to the estimated minimum observable intensity. An E indicates a reflection assumed to be affected by extinction and, consequently, omitted from the final least-squares refinement.

0,0,L		
1	249	259
2	818	-864
3	38*	32
4	971	978
5	228	232
6	129	141
7	330	347
8	451	-451
9	126	-115
10	47*	-49
11	48*	-39
12	48*	13
0,1,L		
1	116	111
2	531	-523
3	24*	4
4	1039	-1036
5	62	-70
6	108	-130
7	158	-164
8	78	-82
9	79	-98
10	41*	39
11	140	-151
12	195	159
0,2,L		
0	148	-168
1	139	148
2	788	-797
3	177	-178
4	51	-57
5	27*	42
6	87	62
7	97	105
8	199	168
9	51	-53
10	40*	-41
11	119	100
0,3,L		
1	32	20
2	992	-1059
3	36*	1
4	426	373
5	175	183
6	275	-278
7	69	-99
8	418	-427
9	84	-114
10	66	101
11	62	-122
0,4,L		
0	77	-39
1	45	-40
2	1069	-1098
3	380	-389
4	138	-109
5	112	-119
6	423	-406
7	79	-93
8	39*	52
9	90	-116
10	103	-83
11	137	182
0,5,L		
1	269	-260
2	935	-918
3	25*	-31
4	526	527
5	353	348
6	114	-116
7	37*	-194
8	196	189
9	75	94
10	41*	168
11	122	-99
0,6,L		
0	451	-438
1	416	405
2	471	-428
3	270	-239
4	435	442
5	77	92
6	239	250
7	171	-166
8	178	154
9	110	-126
10	176	185
11	158	183
0,7,L		
1	265	-263
2	815	824
3	159	-157
4	422	421
5	30*	-4
6	612	610
7	145	120
8	38*	1
9	167	176
10	40*	-41
11	110	100
0,8,L		
0	192	210
1	242	-232
2	772	750
3	503	485
4	406	396
5	91	-94
6	328	-321
7	143	125
8	39*	-24
9	90	-75
10	40*	11
11	45*	6
0,9,L		
1	663	-628
2	193	-162
3	181	172
4	249	-227
5	32*	31
6	261	-262
7	216	-209
8	197	-210
9	194	186
10	43*	-65
11	44*	-11
0,10,L		
0	31*	2
1	164	-194
2	74	64
3	113	-108
4	92	-97
5	188	174
6	86	40
7	89	-72
8	153	-190
9	87	89
10	45*	49
11	44*	-17
0,11,L		
1	406	-387
2	146	133
3	293	307
4	101	-131
5	333	-331
6	142	-147
7	37*	-25
8	65	54
9	90	-93
10	75	-28
0,12,L		
0	30*	48
1	67	-55
2	212	-208
3	39*	42
4	110	-114
5	191	178
6	191	-185
7	48*	84
8	98	-79
9	42*	36
10	69	6
0,13,L		
1	318	305
2	92	-97
3	286	291
4	61	-61
5	133	118
6	39*	-19
7	106	103
8	133	139
9	95	-67
10	264	278
0,14,L		
0	86	74
1	32*	40
2	127	-145
3	186	193
4	111	99
5	354	-350
6	139	133
7	79	-70
8	127	132
9	41*	13
10	46*	-22
0,15,L		
1	669	-645
2	34*	-15
3	273	304
4	37*	30
5	208	-223
6	36*	-5
7	153	-125
8	122	-90
9	146	139
0,16,L		
0	65	56
1	43*	46
2	36*	1
3	215	-203
4	139	46
5	35*	-6
6	66	64
7	40*	7
8	221	215
9	69	-24
0,17,L		
1	151	132
2	36*	2
3	136	-110
4	121	115
5	36*	-13
6	44*	-25
7	73	50
8	88	-70
9	46*	30
0,18,L		
0	75	-43
1	94	82
2	106	-93
3	135	140
4	36*	-19
5	38*	-34
6	181	-158
7	79	-60
8	63	61
0,19,L		
1	35*	-13
2	36*	-24
3	90	-103
4	131	121
5	40*	38
6	110	88
7	143	142
8	45*	-44
0,20,L		
0	36*	-4
1	199	-175
2	68	72
3	56*	23
4	42*	8
5	42*	-26
6	190	-153
7	209	213
0,21,L		
1	104	104
2	72	-39
3	41*	-50
4	44*	53
5	58	73
6	70	52
0,22,L		
0	41*	42
1	165	147
2	198	180
3	41*	-50
4	99	58
5	163	166
6	45*	-6
0,23,L		
1	43*	35
2	43*	-26
3	46*	-65
4	312	-286
5	44*	-26
0,24,L		
0	198	-191
1	104	-84
2	43*	13
3	116	-101
4	47*	40
0,25,L		
1	46*	41
2	45*	48
1,1,L		
0	21*	25
1	69	43
2	445	-447
3	470	-439
4	408	408
5	28*	-21
6	454	466
7	182	-159
8	39*	39
9	89	86
10	79	76
11	71	-41
-1	21*	-40
-2	114	106
-3	218	-201
-4	300	-288
-5	27*	-17
-6	176	183
-7	423	-459
-8	66	72
-9	127	135
-10	40*	14
-11	66	-57
-12	47*	-73
1,2,L		
0	113	103
1	385	401
2	390	399
3	685	-723
4	737	736
5	194	179
6	160	-168
7	34*	-5
8	141	-167
9	60	-77
10	99	-123
11	135	153
-1	586	-609
-2	496	494
-3	646	662
-4	40	-27
-5	101	128
-6	29*	-23
-7	63	57
-8	238	277
-9	35*	-28
-10	92	99
-11	71	-43
-12	117	129
1,3,L		
0	163	165
1	597	628
2	304	-309
3	261	-284
4	409	-412
5	304	274
6	127	-130
7	35*	30
8	161	-182
9	94	-113
10	124	-127
11	67	-46
-1	224	236
-2	95	-93
-3	24*	-23
-4	265	-259
-5	248	242
-6	74	81
-7	165	147
-8	143	-149
-9	36*	-19
-10	98	122
-11	85	92
-12	47*	52
1,4,L		
0	206	-218
1	225	225
2	154	-141
3	114	-130
4	706	681
5	170	180
6	406	-408
7	134	134
8	225	210
9	138	140
10	40*	-33
11	86	88
-1	111	-115
-2	23*	-13
-3	35	20
-4	26*	-25
-5	195	177
-6	314	-325
-7	312	-311
-8	111	-120
-9	211	-250
-10	40*	57
-11	42*	57
1,5,L		
0	95	91
1	32	21
2	79	73
3	291	-304
4	306	-297
5	344	375
6	259	-275
7	50	-65
8	133	-130
9	116	134
10	41*	32
11	44*	21
-1	498	-509
-2	214	210
-3	25*	-21
-4	140	130
-5	212	223
-6	166	163
-7	99	108
-8	250	-278
-9	37*	55
-10	186	206
-11	42*	15
1,6,L		
0	170	-161
1	419	-406
2	512	-495
3	25*	-2
4	209	193
6	224	211
7	323	-345
8	37*	10
9	153	35
10	159	183
11	77	-46
-1	24*	-19
-2	603	-589
-3	37	-1
-4	115	-109
-5	442	-462
-6	279	-281
-7	462	459
-8	150	-128
-9	149	-147
-10	41*	-44
-11	249	273
1,7,L		
0	315	330
1	545	553
2	1275	1282
3	350	-328
4	167	-140
5	752	769
6	198	203
7	390	-409
8	37*	56
9	193	215
10	40*	-11
11	145	-139
-1	213	205
-2	165	165
-3	475	-446
-4	167	176
-5	311	317
-6	131	-124
-7	35*	-26
-8	328	-342
-9	171	-168
-10	39*	3
-11	110	96
1,8,L		
0	233	213
1	512	499
2	755	-734
3	170	-152
4	204	-210
5	144	159
6	533	-499
7	304	-337
8	39*	10
9	194	-164
10	124	-107
11	45*	-7
-1	25*	23
-2	795	763
-3	73	53
-4	321	310
-5	30*	-5
-6	623	641
-7	67	84
-8	35*	-2
-9	107	112
-10	40*	-2
-11	44*	42
1,9,L		
0	455	-459
1	66	82
2	66	-64
3	28*	-34
4	76	70
5	354	-344
6	200	202
7	63	-79
8	174	158
9	94	121
10	148	119
11	76	12
-1	365	-328
-2	166	-162
-3	433	410
-4	131	-143
-5	334	-331
-6	657	635
-7	181	161
-8	147	-161
-9	171	-185
-10	186	180
-11	87	75
1,10,L		
0	471	460
1	151	-158
2	27*	-18
3	161	128
4	192	167
5	124	103
6	149	131
7	38*	-17
8	38*	-20
9	220	230
10	45*	-58
-1	90	77
-2	56	-39
-3	55	-54
-4	303	-294
-5	214	-196
-6	482	496
-7	197	198
-8	127	-133
-9	177	-169
-10	174	149
-11	46*	18
1,11,L		
0	526	-516
1	41	10
2	356	-374
3	119	-117
4	69	-54
5	35*	-53
6	314	-298
7	344	-358
8	112	-119
9	190	232
10	43*	42
-1	204	-214
-2	323	-307
-3	69	68
-4	275	-261
-5	291	-300
-6	72	-80
-7	38*	-71
-8	36*	44
-9	39*	-5
-10	81	99
1,12,L		
0	204	210
1	157	-164
2	52	-54
3	120	-128
4	118	101
5	80	-91
6	161	136
7	78	78
8	53*	-18
9	41*	61
10	165	142
-1	221	228
-2	30*	-42
-3	69	-65
-4	584	-577
-5	55	-31
-6	36*	4
-7	35*	32
-8	158	-179
-9	113	-130
-10	242	-211
1,13,L		
0	150	-162
1	89	82
2	210	-217
3	31*	-6
4	80	83
5	64	78
6	37*	-29
7	37*	31
8	91	88
9	43*	39
10	43*	10
-1	133	142
-2	236	233
-3	90	103
-4	191	-168
-5	105	122
-6	128	104
-7	93	103
-8	125	140
-9	85	-66
-10	123	-125
1,14,L		
0	246	-240
1	119	128
2	289	285
3	174	-159
4	35*	17
5	58	-17
6	83	86
7	206	211
8	93	100
9	69	66
-1	207	-220
-2	253	-259
-3	108	108
-4	438	-425
-5	36*	9
-6	62	-51
-7	76*	10
-8	60	-70
-9	42*	-0
-10	137	165
1,15,L		
0	573	561
1	135	-122
2	437	423
3	297	285
4	425	420
5	181	166
6	85	-98
7	120	126
8	41*	-6
9	44*	-14
-1	35*	28
-2	807	792
-3	63	56
-4	35*	5
-5	82	-89
-6	188	-192
-7	127	104
-8	40*	35
-9	43*	29
1,16,L		
0	45*	-33
1	86	66
2	35*	-8
3	37*	30
4	116	-94
5	58	-52
6	218	-212
7	150	-138
8	116	116
9	83	-101
-1	144	137
-2	485	455
-3	36*	-11
-4	246	226
-5	35*	26
-6	188	201
-7	118	98
-8	42*	-52
-9	43*	12
1,17,L		
0	93	96
1	195	-189
2	536	-534
3	95	-114
4	68	86
5	38*	-33
6	40*	-58
7	39*	-20
8	44*	6
-1	35*	-0
-2	301	-310
-3	58	21
-4	84	62
-5	44*	-69
-6	56	-82
-7	86	69
-8	108	70
-9	46*	45
1,18,L		
0	215	-196
1	40*	38
2	36*	-25
3	36*	16
4	37*	-13
5	68	63
6	136	-156
7	42*	-52
8	46*	-31
-1	107	-108
-2	168	159
-3	33*	11
-4	193	183
-5	110	-90
-6	40*	37
-7	65	61
-8	236	191
1,19,L		
0	39*	-35
1	143	-125
2	213	-203
3	36*	7
4	162	-129
5	60	-77
6	40*	-19
7	46*	53
-1	43*	54
-2	238	-221
-3	57	-71
-4	69	-97
-5	52*	-109
-6	40*	40
-7	78*	27
-8	85	-63
1,20,L		
0	162	-151
1	36*	13
2	60	-21
3	137	132
4	40*	-5
5	59	-27
6	42*	-26
7	43*	-2
-1	161	-161
-2	57	-23
-3	77	95
-4	40*	43
-5	153	-142
-6	203	-161
-7	90*	-30
1,21,L		
0	173	-143
1	64	42
2	111	85
3	41*	54
4	105	101
5	43*	21
6	44*	5
-1	218	192
-2	129	-114
-3	42*	61
-4	207	219
-5	99	-82
-6	137	-80
1,22,L		
0	47*	-21
1	42*	-54
2	45*	-6
3	94	-66
4	485	445
5	83	65
-1	41*	-6
-2	57	45
-3	155	136
-4	432	-407
-5	43*	32
-6	43*	0
1,23,L		
0	218	170
1	66	48
2	101	95
3	43*	-4
4	71	59
5	45*	-13
-1	162	-119
-2	39*	-9
-3	44*	9
-4	42*	17
-5	45*	22
1,24,L		
0	84	45
1	73	-46
2	92	100
3	139	128
-1	45*	-29
-2	42*	-5
-3	145	140
-4	267	213
1,25,L		
0	47*	33
1	79	66
2	67	49
-1	152	-125
-2	43*	26
2,0,L		
0	1800E	2159
1	718	732
2	329	339
3	244	263
4	726	713
5	411	420
6	106	115
7	538	590
8	249	-264
9	329	-353
10	190	211
11	43*	74
2,1,L		
0	827	841
1	486	491
2	167	164
3	497	501
4	291	-277
5	284	-261
6	31*	5
7	149	-148
8	42*	33
9	146	-143
10	75	64
11	162	-140
-1	122	-118
-2	243	228
-3	228	200
-4	1249	1221
-5	276	-265
-6	146	151
-7	57	-44
-8	106	-96
-9	37*	38
-11	41*	33
-12	223	-176
2,2,L		
0	1021	-1015
1	786	-765
2	60	67
3	386	367
4	292	-296
5	358	-350
6	59	41
7	37*	0
8	40*	-25
9	39*	-83
10	120	126
11	44*	61
-1	852	836
-2	227	205
-3	102	-91
-4	329	298
-5	403	377
-6	79	-97
-7	85	-108
-8	72	46
-9	35*	31
-10	95	83
2,3,L		
0	84	-75
1	224	-215
2	99	-102
3	27*	-10
4	55	46
5	94	84
6	105	-117
7	64	-91
8	37*	-2
9	101	-132
10	40*	54
11	161	152
-1	438	406
-2	193	-169
-3	675	-621
-4	554	571
-5	389	354
-6	343	331
-7	106	104
-8	313	283
-9	69	-86
-10	43*	-8
-11	187	197
2,4,L		
0	355	-352
1	229	-228
2	255	-251
3	40	-64
4	211	-217
5	122	-147
6	213	-223
7	37*	-29
8	155	-146
9	38*	1
10	122	-133
11	43*	46
-1	130	-121
-2	544	-488
-3	357	-300
-4	104	-94
-5	53	-55
-6	81	-80
-7	69	-64
-8	220	249
-9	37*	-47
-10	71	82
-11	151	158
2,5,L		
0	82	-79
1	26*	21
2	530	-525
3	25*	-10
4	133	-131
5	181	177
6	330	-330
7	312	-322
8	91	106
9	38*	32
10	42*	31
11	45*	-15
-1	369	346
-2	511	-458
-3	648	-603
-4	64	-73
-5	125	135
-6	59	27
-7	109	-102
-8	349	-336
-9	38*	-54
-10	84	-63
-11	95	93
2,6,L		
0	167	136
1	284	266
2	232	-232
3	252	-241
4	30*	22
5	163	-181
6	409	414
7	72	-135
8	112	121
9	99	120
10	116	95
11	46*	59
-1	411	407
-2	822	-739
-3	95	98
-4	28*	20
-5	30*	-36
-6	412	405
-7	132	-121
-8	39*	-14
-9	153	-142
-10	107	87
-11	72	-66
2,7,L		
0	26*	10
1	373	-362
2	740	710
3	27*	-22
4	100	100
5	164	-158
6	334	357
7	369	363
8	36*	11
9	146	151
10	42*	3
-1	135	-130
-2	917	-841
-3	57	74
-4	168	-167
-5	311	316
-6	622	-601
-7	95	-88
-8	36*	-6
-9	83	-70
-10	78	-62
-11	166	-136
2,8,L		
0	600	577
1	221	-201
2	227	232
3	417	414
4	274	276
5	32*	19
6	39*	-20
7	70	39
8	194	184
9	109	147
10	61	49
-1	186	-181
-2	165	145
-3	209	178
-4	394	-364
-5	447	-453
-6	118	-101
-7	392	397
-8	276	-269
-9	84	-91
-10	232	-204
-11	45*	-22
2,9,L		
0	569	554
1	57	-35
2	40	48
3	150	144
4	32*	42
5	92	91
6	100	123
7	38*	35
8	252	-279
9	39*	14
10	42*	18
-1	469	458
-2	582	547
-3	90	-89
-4	31*	23
-5	77	92
-6	281	263
-7	38*	-3
-8	92	98
-9	128	-98
-10	41*	-11
-11	43*	-33
2,10,L		
0	313	311
1	126	117
2	54	-45
3	154	-165
4	408	-393
5	114	128
6	42*	3
7	66	-78
8	200	-239
9	104	98
10	45*	-2
-1	27*	-16
-2	231	231
-3	203	-194
-4	91	86
-5	197	168
-6	385	340
-7	91	88
-8	37*	-32
-9	39*	1
-10	41*	-16
-11	44*	5
2,11,L		
0	29*	10
1	190	-177
2	152	-164
3	51	-71
4	34*	-13
5	294	-303
6	213	119
7	37*	34
8	96	-124
9	109	-125
10	45*	17
-1	30*	36
-2	306	280
-3	117	-122
-4	171	-168
-5	234	207
-6	204	192
-7	152	-179
-8	139	119
-9	341	314
-10	43*	-26
2,12,L		
0	33*	58
1	30*	-17
2	126	-139
3	56	-72
4	97	-96
5	255	243
6	244	-233
7	37*	-27
8	97	-126
9	42*	-5
10	45*	4
-1	124	111
-2	154	124
-3	138	-119
-4	35*	54
-5	248	240
-6	38*	-15
-7	177	180
-8	72	-36
-9	41*	-9
-10	133	121
2,13,L		
0	755	-723
1	287	272
2	261	-231
3	35*	-16
4	512	-475
5	249	175
6	137	141
7	40*	34
8	38*	-12
9	157	-142
-1	112	-96
-2	290	268
-3	247	-230
-4	327	-300
-5	186	-181
-6	38*	56
-7	134	-139
-8	40*	28
-9	119	129
-10	190	-174
2,14,L		
0	536	-527
1	34*	20
2	50	-25
3	65	-66
4	462	416
5	40*	-40
6	38*	50
7	59	-59
8	120	97
9	41*	-18
-1	33*	26
-2	190	172
-3	36*	-44
-4	460	-419
-5	226	-181
-6	36*	26
-7	269	-248
-8	40*	17
-9	66	-81
-10	43*	-14
2,15,L		
0	249	233
1	453	-441
2	37*	-40
3	211	222
4	41*	18
5	93	-63
6	101	117
7	99	-86
8	211	-186
9	46*	61
-1	635	594
-2	73	-75
-3	143	-148
-4	37*	-6
-5	36*	53
-6	35*	11
-7	163	145
-8	70	-46
-9	128	-95
2,16,L		
0	215	-203
1	305	-285
2	42*	90
3	97	-50
4	74	91
5	36*	15
6	105	115
7	113	-121
8	44*	26
-1	304	284
-2	89	78
-3	231	-212
-4	37*	-61
-5	172	144
-6	38*	8
-7	57	-78
-8	76	-49
-9	108	-72
2,17,L		
0	77	-91
1	166	-124
2	579	556
3	35*	18
4	37*	8
5	72	49
6	39*	37
7	42*	8
8	169	131
-1	38*	13
-2	233	189
-3	36*	-24
-4	125	108
-5	89	48
-6	37*	-22
-7	42*	48
-8	43*	30
2,18,L		
0	134	-139
1	84	-79
2	51	-28
3	199	215
4	39*	19
5	42*	51
6	41*	-27
7	215	-209
-1	164	164
-2	233	224
-3	168	157
-4	129	-136
-5	68	25
-6	140	123
-7	44*	-44
-8	73	34
2,19,L		
0	77	-67
1	122	-110
2	179	160
3	149	129
4	60	40
5	86	-114
6	122	-124
7	159	113
-1	37*	31
-2	104	-91
-3	38*	32
-4	40*	-31
-5	38*	18
-6	214	-213
-7	152	-124
2,20,L		
0	89	98
1	236	-227
2	61	-43
3	176	144
4	164	-138
5	41*	-19
6	155	-145
-1	100	-93
-2	262	227
-3	40*	33
-4	41*	-52
-5	123	-109
-6	224	213
-7	160	141
2,21,L		
0	275	-244
1	129	-95
2	160	-123
3	138	141
4	43*	1
5	268	-224
6	181	-158
-1	158	-149
-2	89	-61
-3	39*	0
-4	42*	-1
-5	43*	27
-6	44*	-23
2,22,L		
0	45*	50
1	200	171
2	242	201
3	43*	-42
4	46*	-47
5	207	147
-1	41*	17
-2	66	-30
-3	92	-96
-4	184	-142
-5	77	49
2,23,L		
0	43*	-0
1	45*	57
2	43*	-2
3	318	258
4	48*	-56
-1	43*	29
-3	173	135
-4	252	214
2,24,L		
0	124	-98
1	85	83
2	46*	54
3	309	-251
-1	80	-67
-2	42*	-4
-3	43*	-8
2,25,L		
0	46*	30
-1	47*	-49
3,1,L		
0	1014	-977
1	298	-300
2	503	496
3	29*	20
4	86	82
5	196	-183
6	88	113
7	155	-144
8	163	172
9	188	210
10	126	131
-1	26*	49
-2	329	-311
-3	141	-127
-4	306	-300
-5	31*	-26
-6	114	-111
-7	267	-278
-8	226	-135
-9	42*	-69
-10	39*	43
-11	104	-97
3,2,L		
0	868	843
1	37	-6
2	800	814
3	181	-165
4	276	303
5	62	-40
6	187	199
7	279	264
8	68	68
9	38*	-16
10	122	-128
-1	224	-211
-2	273	273
-3	158	155
-4	110	-110
-5	135	153
-6	58	59
-7	54	46
-8	159	16
-9	36*	19
-10	161	-157
-11	182	-202
3,3,L		
0	109	-80
1	241	224
2	381	362
3	210	205
4	203	-219
5	52	-59
6	208	-204
7	202	59
8	35*	10
9	69	-110
10	143	-172
-1	86	-79
-2	446	423
-3	226	212
-4	130	135
-5	213	198
-6	345	343
-7	207	203
-8	88	-77
-9	39*	75
-10	159	167
-11	45*	53
3,4,L		
0	578	519
1	27*	5
2	99	111
3	280	274
4	45	-49
5	64	-103
6	160	-160
7	227	219
8	202	198
9	137	136
10	113	-145
-1	138	145
-2	799	-737
-3	165	-158
-4	125	109
-5	111	117
-6	280	-281
-7	139	-146
-8	46*	-114
-9	39*	-53
-10	40*	-4
-11	147	-156
3,5,L		
0	258	245
1	180	162
2	218	-228
3	30*	-5
4	71	-80
5	135	131
6	412	-410
7	43*	55
8	38*	-47
9	40*	-38
10	90	-100
-1	204	-195
-2	859	827
-3	28*	18
-5	123	131
-6	174	152
-7	122	-130
-8	139	100
-9	178	189
-10	64	-45
-11	147	-135
3,6,L		
0	67	41
1	206	-202
2	724	-730
3	87	-94
4	377	-382
5	367	-357
6	67	69
7	83	93
8	64	-42
9	138	-157
10	42*	-12
-1	165	-182
-2	874	-830
-3	33*	-31
-4	29*	4
-5	176	-155
-6	216	226
-7	329	335
-8	66	-62
-9	38*	7
-10	87	84
-11	113	108
3,7,L		
0	359	346
1	60	-47
2	29*	15
3	76	82
4	32*	-37
5	193	201
6	419	428
7	69	71
8	38*	11
9	40*	45
10	94	61
-1	130	-120
-2	388	-358
-3	248	-236
-4	211	-210
-5	121	-133
-6	417	-417
-7	43*	40
-8	130	-113
-9	40*	72
-10	156	-185
-11	92	80
3,8,L		
0	29*	-6
1	654	673
2	91	-90
3	98	-87
4	162	-155
5	148	160
6	141	-122
7	236	-225
8	77	91
9	224	-242
10	166	-162
-1	203	192
-2	148	153
-3	199	-191
-4	479	504
-5	34*	39
-6	38*	44
-7	229	-139
-8	172	170
-9	40*	4
-10	80	-46
-11	139	153
3,9,L		
0	55	43
1	29*	21
2	512	-500
3	165	-172
4	346	382
5	330	-314
6	75	-50
7	67	61
8	162	168
9	59	-37
10	47*	-83
-1	222	221
-2	30*	16
-3	252	261
-4	360	-393
-5	65	-58
-6	314	307
-7	46*	-74
-8	38*	46
-9	65	-45
-10	43*	-52
-11	44*	-56
3,10,L		
0	246	238
1	165	153
2	30*	5
3	119	-139
4	486	499
5	74	93
6	95	80
7	204	179
8	96	97
9	43*	4
-1	287	-285
-2	206	207
-3	180	168
-4	35*	27
-5	37*	47
-6	116	154
-7	35*	-28
-8	86	-112
-9	154	-120
-10	130	130
3,11,L		
0	31*	12
1	251	-231
2	291	-287
3	62	-91
4	128	132
5	153	84
6	67	-85
7	123	-142
8	178	-163
9	125	109
-1	101	100
-2	218	-210
-3	33*	-46
-4	69	-76
-5	209	-228
-6	192	56
-7	100	99
-8	232	229
-9	41*	-20
-10	139	100
3,12,L		
0	100	107
1	34*	50
2	119	-119
3	180	-201
4	196	207
5	44*	98
6	104	-118
7	76	51
8	112	-142
9	149	-135
-1	239	-222
-2	34*	-39
-3	124	129
-4	159	-166
-5	150	-166
-6	316	-339
-7	60	53
-8	41*	-42
-9	201	-164
-10	87	-65
3,13,L		
0	39*	-28
1	100	-94
2	37*	17
3	37*	-10
4	165	-28
5	35*	23
6	84	-106
7	120	-116
8	91	96
9	45*	-35
-1	498	475
-2	56	41
-3	213	-223
-4	138	138
-5	288	259
-6	34*	19
-7	68	64
-8	87	-17
-9	236	-225
-10	104	-93
3,14,L		
0	388	-371
1	38*	-46
2	37*	8
3	45*	-102
4	40*	-67
5	36*	8
6	159	-157
7	121	111
8	44*	57
-1	370	-354
-2	156	-148
-3	445	474
-4	169	-156
-5	51	-68
-6	169	-170
-7	150	161
-8	42*	57
-9	43*	24
3,15,L		
0	80	57
1	255	-248
2	305	303
3	359	369
4	105	107
5	213	225
6	102	-90
7	76	65
8	43*	32
-1	98	97
-2	302	299
-3	373	-381
-4	38*	0
-5	36*	57
-6	117	-97
-7	127	114
-8	138	-133
-9	47*	-32
3,16,L		
0	277	226
1	151	56
2	60	99
3	212	219
4	102	96
5	39*	-7
6	39*	-8
7	161	-164
8	199	182
-1	184	108
-2	242	191
-3	40*	71
-4	251	221
-5	272	-278
-6	106	95
-7	89	62
-8	104	-55
-9	66	-32
3,17,L		
0	36*	42
1	36*	-14
2	163	-162
3	36*	-16
4	71	-49
5	185	-160
6	42*	3
7	46*	-61
-1	36*	2
-2	156	-171
-3	36*	50
-4	111	87
-5	123	132
-6	83	51
-7	43*	-52
-8	119	-121
3,18,L		
0	35*	13
1	63	-69
2	63	-78
3	39*	28
4	71	-92

Table 2 (*cont.*)

3,18,L		
	125	-132
	44*	-15
	45*	-41
	36*	-21
-2	126	-112
-3	109	106
-4	188	182
-5	183	-189
-6	117	97
-7	240	236
-8	195	183
3,19,L		
0	45*	25
1	114	-117
2	39*	-46
3	107	117
4	73	-64
5	147	-174
6	45*	46
-1	37*	-5
-2	79	-72
-3	172	-159
-4	70	-62
-5	138	143
-6	172	162
-7	173	-179
3,20,L		
0	48*	-41
1	39*	17
2	144	-148
3	188	186
4	76	-53
5	220	-222
6	169	-145
-1	88	-75
-2	108	-103
-3	40*	-4
-4	73	-51
-5	150	-131
-6	43*	-26
3,21,L		
0	45*	-28
1	109	-108
2	66	-61
3	128	110
4	45*	73
5	132	-140
-1	216	192
-2	120	-110
-3	73	78
-4	42*	1
-5	132	-111
-6	98	-69
3,22,L		
0	62	67
1	41*	-10
2	44*	33
3	152	-126
4	277	269
-1	145	110
-2	42*	20
-3	140	-119
-4	278	-239
-5	205	194
3,23,L		
0	146	117
1	42*	-7
2	92	-87
3	74	-52
-1	43*	4
-2	43*	-11
-3	135	-117
-4	116	-92
3,24,L		
0	45*	3
1	43*	-22
-1	45*	-22
-2	143	115
4,0,L		
0	225	204
1	431	432
2	242	227
3	183	176
4	351	-377
5	186	225
6	78	-48
7	300	339
8	137	149
9	43*	-45
10	80	-52
4,1,L		
0	266	257
1	563	590
2	108	111
3	252	305
4	172	198
5	130	-134
6	236	250
7	63	73
8	80	84
9	158	-165
10	92	113
-1	396	-385
-2	299	290
-3	180	174
-4	164	152
-5	455	-472
-6	97	105
-7	242	-281
-8	61	-57
-9	172	168
-10	115	-120
-11	45*	-54
4,2,L		
0	30*	1
1	398	-382
2	115	107
3	477	495
4	141	-142
5	432	-461
6	57	-29
7	98	-110
8	87	77
9	43*	70
10	44*	8
-1	536	531
-2	30*	23
-3	184	193
-4	112	106
-5	145	-158
-6	54	14
-7	48*	133
-8	36*	-5
-9	79	-77
-10	134	-128
4,3,L		
0	62	86
1	98	-118
2	277	-264
3	85	-81
4	150	-148
5	241	-263
6	308	330
7	108	131
8	41*	-71
9	139	-176
10	45*	52
-1	382	366
-2	29*	-15
-3	141	-143
-4	31*	0
-5	254	250
-6	306	304
-7	44*	-95
-8	125	128
-9	107	98
-10	40*	-7
-11	45*	1
4,4,L		
0	166	-149
1	306	-312
2	142	150
3	43	18
4	186	171
5	35*	-31
6	164	-170
7	90	98
8	70	61
9	101	87
10	106	-123
-1	62	-12
-2	63	75
-3	110	-120
-4	104	117
-5	71	-59
-6	107	-100
-7	227	177
-8	433	434
-9	191	-215
-10	43*	-27
-11	216	190
4,5,L		
0	159	-160
1	204	197
2	313	-312
3	129	-120
4	430	-442
5	85	78
6	39*	49
7	96	-113
8	182	-201
9	82	-82
10	68	-83
-1	117	101
-2	30*	10
-3	365	-361
-4	285	-279
-5	144	130
-6	205	201
-7	302	-263
-8	35*	-17
-9	297	297
-10	69	63
-11	43*	-27
4,6,L		
0	156	-160
1	64	74
2	216	-225
3	157	-180
4	364	364
5	160	-190
6	36*	-11
7	61	-18
8	41*	36
9	44*	-57
-1	265	268
-2	269	-277
-3	122	126
-4	85	-63
-5	126	117
-6	160	-165
-7	270	-287
-8	206	214
-9	88	-101
-10	40*	-43
-11	46*	-25
4,7,L		
0	33*	-55
1	291	-305
2	610	617
3	59	45
4	197	-195
5	108	-141
6	141	151
7	352	380
8	41*	-1
9	99	115
-1	175	-173
-2	75	-65
-3	217	238
-4	34*	-9
-5	126	125
-6	449	-427
-7	36*	21
-8	37*	27
-9	41*	42
-10	43*	-10
4,8,L		
0	32*	-40
1	408	-410
2	490	-485
3	224	230
4	472	480
5	96	45
6	257	-268
7	39*	56
8	149	160
9	45*	-38
-1	105	-109
-2	57	71
-3	57	-38
-4	309	-316
-5	218	-214
-6	354	-358
-7	206	220
-8	40*	-45
-9	40*	25
-10	265	-254
4,9,L		
0	114	125
1	137	147
2	449	435
3	87	104
4	37*	28
5	183	214
6	127	136
7	48*	13
8	43*	52
9	44*	5
-1	67	76
-2	162	136
-3	88	-80
-4	37*	50
-5	35*	-31
-6	143	-75
-7	42*	4
-8	205	-189
-9	106	-96
-10	44*	41
4,10,L		
0	321	315
1	34*	62
2	117	-67
3	210	219
4	111	-124
5	35*	13
6	39*	-29
7	41*	42
8	148	-150
9	64	-101
-1	166	186
-2	215	206
-3	36*	-44
-4	517	498
-5	101	97
-6	40*	59
-7	59	-59
-8	138	151
-9	42*	-6
-10	45*	-40
4,11,L		
0	290	-282
1	36*	52
2	195	201
3	228	-230
4	41*	14
5	136	-148
6	129	-143
7	114	-147
8	81	73
-1	274	-259
-2	52	57
-3	36*	38
-4	246	224
-5	210	161
-6	52	-51
-7	121	-136
-8	185	158
-9	170	146
-10	44*	-2
4,12,L		
0	509	500
1	38*	18
2	64	-66
3	102	39
4	38*	12
5	112	100
6	68	-84
7	40*	-21
8	42*	9
-1	35*	-25
-2	54	-46
-3	78	75
-4	396	379
-5	37*	26
-6	38*	35
-7	166	162
-8	44*	-37
-9	98	77
4,13,L		
0	704	-702
1	309	288
2	39*	-8
3	37*	15
4	454	-456
5	38*	42
6	77	-51
7	122	-144
8	45*	37
-1	112	-105
-2	36*	19
-3	40*	59
-4	111	115
-5	68	-60
-6	123	99
-7	40*	-43
-8	104	85
-9	44*	4
4,14,L		
0	387	-403
1	110	-28
2	38*	22
3	226	-232
4	39*	18
5	38*	7
6	41*	43
7	42*	-44
8	224	199
-1	40*	-41
-2	297	-250
-3	129	-138
-4	457	-446
-5	161	-149
-6	39*	33
-7	100	-63
-8	74	-50
-9	186	-179
4,15,L		
0	312	301
1	129	82
2	116	-127
3	37*	-10
4	143	126
5	41*	40
6	43*	82
7	44*	-15
-1	38*	-43
-2	194	-184
-3	71	86
-4	38*	-36
-6	41*	37
-7	40*	-11
-8	152	-102
4,16,L		
0	158	157
1	37*	35
2	39*	-27
3	155	-130
4	91	-77
5	58	-32
6	43*	65
7	46*	-43
-1	35*	38
-2	391	-365
-3	37*	-36
-4	96	-64
-5	38*	36
-6	41*	44
-7	86	82
-8	247	-213
4,17,L		
0	93	70
1	121	-125
2	365	340
3	69	35
4	97	-20
5	41*	38
6	191	200
-1	39*	-68
-2	232	228
-3	55	27
-4	72	-51
-5	41*	-42
-6	41*	-2
-7	43*	6
-8	136	-98
4,18,L		
0	62	53
1	171	160
2	69	64
3	95	-38
4	59	57
5	86	101
6	81	67
-1	76	75
-2	253	225
-3	72	70
-4	98	-45
-5	104	77
-6	258	244
-7	166	139
4,19,L		
0	43*	6
1	39*	7
2	58	55
3	42*	0
4	42*	-4
5	45*	28
-1	42*	26
-2	102	87
-3	41*	38
-4	294	-263
-5	43*	-23
-6	83	-108
4,20,L		
0	160	146
1	139	91
2	145	-149
3	42*	-7
4	49*	52
-1	150	-143
-2	319	283
-3	62*	-10
-4	48*	-20
-5	129	-96
-6	242	196
4,21,L		
0	234	-206
1	136	-121
2	236	-198
3	71	-66
4	155	-127
-1	44*	42
-2	159	138
-3	43*	-24
-4	101	-71
-5	47*	-21
4,22,L		
0	16*	-142
1	80	68
2	44*	-15
-1	136	-109
-2	84	-78
-3	46*	-42
-4	112	-80
4,23,L		
0	110	-112
-1	149	116
-2	68	49
5,1,L		
0	220	-232
1	80	-93
2	237	-264
3	217	-228
4	57	51
5	39*	-3
6	38*	60
7	136	-124
8	42*	-15
9	212	271
-1	200	-170
-2	199	-219
-3	323	308
-4	687	-686
-5	460	-452
-6	36*	22
-7	160	174
-8	38*	-30
-9	148	-142
-10	43*	-21
5,2,L		
0	35*	20
1	117	-108
2	380	414
3	93	-81
4	217	246
5	38*	53
6	57	96
7	179	229
8	41*	20
9	79	-56
-1	223	-219
-2	529	541
-3	35*	-54
-4	351	-356
-5	92	98
-6	257	-260
-7	122	-108
-8	39*	-39
-9	40*	23
-10	270	-242
5,3,L		
0	102	108
1	240	257
2	244	255
3	35*	21
4	113	129
5	38*	46
6	70	-86
7	39*	-23
8	169	190
9	44*	7
-1	153	-162
-2	653	654
-3	362	354
-4	57	-49
-5	99	-118
-6	405	420
-7	295	294
-8	83	-66
-9	41*	5
-10	71	52
5,4,L		
0	79	-78
1	34*	-13
2	49	44
3	224	246
4	156	168
5	52	60
6	38*	-50
7	134	143
8	43*	-45
9	70	30
-1	124	-105
-2	152	146
-3	215	218
-4	61	-54
-5	37*	-47
-6	324	-326
-7	84	-82
-8	39*	27
-9	118	114
-10	69	56
5,5,L		
0	93	-89
1	234	236
2	140	165
3	60	45
4	38*	-10
5	277	295
6	295	-333
7	165	-175
8	104	114
9	46*	3
-1	33*	42
-2	568	574
-3	50	-49
-4	339	339
-5	140	-130
-6	39*	-49
-7	36*	2
-8	131	144
-9	43*	-67
-10	50*	-58
5,6,L		
0	231	-207
1	62	-54
2	256	-282
3	102	-126
4	195	-201
5	263	-289
6	91	-112
7	99	82
8	140	-146
9	157	-190
-1	66	-76
-2	140	141
-3	194	207
-4	109	103
-5	37*	-0
-6	280	286
-7	38*	17
-8	125	112
-9	86	95
-10	200	203
5,7,L		
0	396	-392
1	161	-180
2	35*	12
3	107	107
4	157	-181
5	84	-109
6	39*	5
7	78	93
8	69	73
-1	319	-334
-2	257	-271
-3	35*	-4
-4	36*	19
-5	82	-82
-6	237	-227
-7	138	163
-8	156	-159
-9	42*	33
-10	70	47
5,8,L		
0	230	-235
1	153	140
2	116	126
3	106	138
4	270	-286
5	38*	-40
6	222	228
7	133	-135
8	44*	57
-1	67	61
-2	350	-361
-3	36*	7
-4	312	327
-5	236	-252
-6	165	-176
-7	40*	-10
-8	142	149
-9	43*	26
-10	46*	41
5,9,L		
0	208	-197
1	36*	45
2	79	82
3	73	-21
4	197	207
5	98	-98
6	189	-193
7	96	-80
8	76	122
-1	153	158
-2	101	-76
-3	96	111
-4	123	-143
-5	115	130
-6	37*	-7
-7	182	-168
-8	80	-58
-9	105	-95
5,10,L		
0	203	217
1	80	79
2	154	149
3	36*	-29
4	126	135
5	112	-81
6	42*	29
7	131	127
8	212	238
-1	107	-101
-2	149	-142
-3	69	84
-4	133	111
-5	91	97
-6	54	-55
-7	126	-106
-8	193	-190
-9	45*	-9
5,11,L		
0	63	82
1	91	-89
2	39*	15
3	58	-69
4	126	145
5	38*	35
6	115	123
7	44*	53
-1	137	-173
-2	38*	21
-3	117	100
-4	94	-98
-5	36*	-61
-6	179	192
-7	38*	-6
-8	42*	24
-9	43*	11
5,12,L		
0	354	343
1	76	112
2	38*	21
3	35*	34
4	39*	-20
5	40*	-19
6	98	-75
7	181	195
-1	287	-263
-2	265	-266
-3	72	16
-4	157	141
-5	145	-145
-6	111	-106
-7	170	169
-8	41*	15
-9	73	-88
5,13,L		
0	201	198
1	115	115
2	41*	28
3	79	-59
4	68	-65
5	40*	-53
6	113	91
7	133	-105
-1	98	116
-2	44*	-45
-3	36*	-20
-4	76	60
-5	38*	39
-6	39*	25
-7	42*	-23
-8	71	-77
5,14,L		
0	87	-78
1	37*	-22
2	56	18
3	38*	-9
4	46*	-113
5	133	-133
6	243	-250
7	110	101
-1	96	-112
-2	36*	-23
-3	228	251
-4	40*	51
-5	112	100
-6	124	-125
-7	140	132
-8	150	132
5,15,L		
0	63	-18
1	37*	-7
2	170	-171
3	63	70
4	231	-211
5	181	182
6	44*	-4
-1	57	-26
-2	110	115
-3	120	-120
-4	97	-81
-5	46*	-33
-6	107	109
-7	194	203
-8	45*	-5
5,16,L		
0	94	61
1	41*	46
2	40*	-16
3	115	102
4	200	182
5	46*	30
6	46*	78
-1	38*	28
-2	39*	-4
-3	172	-175
-4	63	59
-5	153	-127
-6	45*	-50
-7	88	-93
5,17,L		
0	81	71
1	269	270
2	39*	11
3	205	-179
4	121	-68
5	45*	0
-1	107	-106
-2	40*	-16
-3	155	156
-4	66	-61
-5	122	-106
-6	45*	-3
-7	47*	-20
5,18,L		
0	127	-92
1	42*	-7
2	130	-112
3	93	-111
4	43*	-27
-1	40*	-1
-2	43*	2
-3	169	174
-4	41*	-4
-5	44*	-46
-6	45*	20
5,19,L		
0	46*	23
1	43*	-32
2	163	147
3	82	-69
4	46*	-59
-1	53	-60
-2	42*	-19
-3	96	-93
-4	74	97
-5	45*	47
5,20,L		
0	127	-115
1	45*	34
2	122	-102
3	91	75
-1	41*	-16
-2	149	127
5,21,L		
0	139	-112
1	76	-76
-1	103	99
-2	83	-74
-3	94	74
6,0,L		
0	357	-384
1	124	124
2	203	-224
3	117	90
4	335	-396
5	104	96
6	123	-149
7	119	125
8	72	-73
6,1,L		
0	441	-489
1	257	287
2	142	145
3	38*	15
4	109	123
5	56	47
6	81	83
7	41*	31
8	151	175
-1	313	-355
-2	146	153
-3	38*	32
-4	103	-124
-5	297	-301
-6	43*	-1
-7	160	-167
-8	75	54
-9	73	72
-10	47*	-54
6,2,L		
0	36*	15
1	154	-142
2	69	-83
3	202	225
4	201	241
5	145	-162
6	43*	61
7	64	-71
8	47*	-95
-1	236	255
-2	243	227
-3	38*	35
-4	173	-196
-5	130	-150
-6	86	-68
-7	85	-94
-8	115	105
-9	45*	49
-10	186	-190
6,3,L		
0	295	-259
1	61	46
2	37*	-14
3	127	-156
4	36*	17
5	185	-194
6	40*	-28
7	43*	-61
8	44*	7
-1	37*	59
-2	132	-136
-3	114	132
-4	67	39
-5	162	171
-6	63	-54
-7	117	-98
-8	76	-82
-9	44*	-33
-10	82	110
6,4,L		
0	39*	-16
1	340	-369
2	267	287
3	37*	39
4	39*	28
5	39*	30
6	91	101
7	45*	86
8	46*	52
-1	106	114
-2	111	122
-3	106	-138
-4	57	10
-5	38*	-28
-6	62	-48
-7	154	153
-8	78	58
-9	198	-196
6,5,L		
0	386	-390
1	126	165
2	212	193
3	82	-75
4	202	-227
5	167	200
6	41*	5
7	160	-199
8	89	-107
-1	57	-66
-2	208	199
-3	64	-103
-4	149	153
-5	129	110
-6	81	116
-7	126	-124
-8	119	99
-9	112	106
6,6,L		
0	182	-194
1	40*	-18
2	286	300
3	60	-58
4	129	-145
5	110	-120
6	116	125
7	61	-22
-1	195	220
-2	220	-245
-3	102	-71
-4	103	-113
-5	221	211
-6	56	-36
-7	199	-203
-8	44*	48
-9	45*	18
6,7,L		
0	41*	34
1	172	-190
2	382	412
3	215	218
4	39*	-10
5	40*	-30
6	43*	-77
7	130	149
-1	151	-145
-2	309	296
-3	279	291
-4	62	58
-5	88	-101
-6	219	-210
-7	90	74
-8	43*	-24
-9	43*	-29
6,8,L		
0	165	-168
1	226	-257
2	128	-100
3	96	104
4	181	-188
5	43*	-54
6	81	-101
7	45*	-15
-1	64	20
-2	41*	-3
-3	189	-187
-4	170	-192
-5	39*	40
-6	139	133
-7	175	168
-8	170	-179
-9	47*	68
6,9,L		
0	37*	29
1	37*	13
2	35*	-31
3	89	91
4	39*	-11
5	42*	71
6	135	150
7	44*	9
-1	72	-87
-2	38*	-66
-3	40*	-36
-4	308	-287
-5	89	-95
-6	39*	-0
-7	43*	-6
-8	257	-239
-9	121	131
6,10,L		
0	37*	6
1	96	107
2	218	255
3	368	384
4	252	-264
5	193	-206
6	130	153
7	133	152
-1	137	148
-2	106	83
-3	64	-53
-4	274	266
-5	80	63
-6	123	112
-7	150	-141
-8	45*	-2
6,11,L		
0	42*	-29
1	73	-65
3	137	-123
4	41*	-25
5	143	-162
6	46*	-36
-1	37*	-28
-2	41*	30
-3	38*	5
-4	38*	-18
-5	41*	49
-6	42*	-27
-7	101	-84
-8	264	262
6,12,L		
0	142	159
1	179	171
3	43*	-17
4	45*	47
5	41*	-39
6	49*	40
-1	217	-240
-2	223	229
-3	89	98
-4	178	169
-5	42*	28
-6	44*	-12
-7	60	-52
-8	75	27
6,13,L		
0	119	-136
1	118	114
2	41*	-39
3	75	90
4	201	-206
5	117	-125
6	76	64
-1	214	187
-2	55	36
-3	40*	32
-4	101	99
-5	42*	4
-6	160	165
-7	79	-75
6,14,L		
0	427	-454
1	51*	-128
2	39*	14
3	132	-145
4	45*	-54
5	42*	-40
-1	38*	6
-2	40*	-0
-3	61	-79
-4	316	-323
-5	42*	28
-6	115	-110
-7	133	-125
6,15,L		
0	136	132
1	103	128
2	41*	-28
3	160	-193
4	45*	17
5	73	87
-1	40*	-65
-2	185	-172
-3	119	-107
-4	58	26
-5	106	95
-6	100	-69
6,16,L		
0	44*	56
1	135	140
2	113	-109
3	107	-111
4	44*	14
-1	201	-180
-2	199	-178
-3	198	188
-4	44*	-28
-5	46*	-47
-6	166	-149
6,17,L		
0	43*	-9
1	90	-79
2	174	175
3	45*	35
-1	41*	-3
-2	42*	27
-3	116	-91
-4	46*	70
-5	46*	41
6,18,L		
0	145	114
1	43*	-9
2	67	65
-1	88	93
-2	147	125
-3	134	108
-4	117	103
6,19,L		
0	95	-71
1	46*	62
-1	63	-17
-2	46*	31
-3	44*	-13
7,1,L		
0	44*	-6
1	83	-83
2	223	-242
4	162	159
5	44*	23
6	116	-131
-1	86	-74
-2	279	-292
-3	70	83
-4	62	-49
-5	43*	-44
-6	182	-182
-7	42*	46
-8	69	47
-9	116	-135
7,2,L		
0	38*	-47
1	114	-111
2	114	132
3	40*	-5
4	42*	-69
5	44*	78
6	91	-89
-1	91	-79
-2	37*	-4
-3	181	-185
-4	121	-121
-5	41*	-3
-6	188	-190
-7	102	108
-8	133	-114
7,3,L		
0	107	86
1	43*	39
2	115	116
3	39*	21
4	199	214
5	43*	-30
6	97	-96
-1	37*	-5
-2	240	263
-3	39*	6
-4	122	109
-5	76	95
-6	43*	79
-7	41*	-4
-8	45*	-27
7,4,L		
0	66	78
1	38*	49
2	85	69
3	136	146
4	137	136
5	116	119
6	46*	-76
-1	81	-91
-2	38*	-19
-3	162	166
-5	135	-121
-6	104	-39
-7	211	207
-8	71	-83
7,5,L		
0	39*	61
1	141	123
2	40*	-4
3	105	123
4	82	-57
5	94	119
6	45*	37
-1	72	92
-2	39*	32
-3	38*	-16
-4	172	152
-5	225	-232
-6	42*	-67
-7	62	64
-8	134	134
7,6,L		
0	92	99
1	40*	48
2	51*	47
3	42*	-77
4	42*	-17
5	45*	-70
6	128	-166
-1	43*	50
-2	39*	56
-3	41*	42
-4	208	218
-5	42*	-16
-6	196	186
-7	45*	20
-8	113	99
7,7,L		
0	41*	-38
1	75	-87
2	126	-133
3	79	87
4	213	-234
5	239	-279
6	45*	-26
-2	39*	-7
-3	121	120
-4	40*	-22
-5	83	-74
-6	144	134
-7	109	115
-8	63	-18
7,8,L		
0	230	-231
1	74	-87
2	109	-130
3	59	72
4	82	-102
5	185	-209
6	136	138
-1	41*	-66
-2	296	-301
-3	122	110
-4	41*	38
-5	186	-198
-6	93	-86
-7	100	117
-8	173	176
7,9,L		
0	41*	28
1	42*	15
2	96	88
3	42*	42
4	45*	-28
5	47*	-51
-1	40*	64
-2	146	-152
-3	109	60
-4	168	-175
-5	42*	-31
-6	43*	-17
-7	46*	-24
7,10,L		
0	105	77
1	41*	30
2	101	-86
3	43*	0
4	177	175
5	43*	-17
-1	41*	64
-2	40*	-1
-3	41*	12
-4	43*	-44
-5	84	127
-6	258	-267
-7	207	-201
7,11,L		
0	41*	-0
1	71	-56
2	142	109
3	99	-121
4	44*	17
5	46*	-25
-1	44*	-90
-2	59	76
-3	42*	-54
-4	138	-125
-5	45*	54
-6	47*	-34
-7	86	-81
7,12,L		
0	215	201
1	42*	33
2	141	-135
3	67	77
4	110	121
-1	136	-134
-2	136	106
-3	41*	-2
-4	62	49
-5	43*	-56
-6	45*	23
7,13,L		
0	43*	0
1	79	68
2	136	155
3	46*	5
4	45*	38
-1	42*	-4
-2	79	-88
-3	44*	-32
-4	213	208
-5	46*	28
-6	179	-181
7,14,L		
0	121	112
1	170	-160
2	43*	22
3	85	69
-1	141	138
-2	80	111
-3	44*	49
-4	79	73
-5	44*	26
7,15,L		
0	167	-146
1	44*	-18
-1	103	114
-2	87	97
-3	43*	-11
-4	281	259
7,16,L		
0	53*	27
1	87	-105
-1	85	92
-2	303	-288
-3	161	-189
7,17,L		
-1	130	-118
-2	48*	-35
8,0,L		
0	47*	-73
1	128	131
2	44*	-1
3	156	165
4	307	-375
5	46*	-58
8,1,L		
0	308	-390
1	43*	27
2	42*	-25
3	44*	-10
4	87	-93
5	64	-0
-1	65	-71
-2	65	63
-3	44*	35
-4	156	-153
-5	132	-141
-6	126	127
-7	47*	22
8,2,L		
0	44*	33
1	43*	-8
2	67	25
3	42*	8
4	78	129
5	45*	-8
-1	43*	58
-2	154	-142
-3	192	-163
-4	63	3
-5	44*	13
-6	73	-48
-7	49*	-81
8,3,L		
0	79	117
1	127	115
2	160	-163
3	164	-176
4	46*	39
-1	43*	-51
-2	275	-284
-3	147	159
-4	146	-146
-5	45*	3
-6	44*	-20
-7	45*	10
8,4,L		
0	101	119
1	77	-102
2	44*	28
3	79	-71
4	46*	15
-1	44*	-72
-2	136	-85
-3	66	-60
-4	86	-30
-5	42*	-10
-6	136	-133
-7	48*	29
8,5,L		
0	102	61
1	70	44
2	42*	37
3	92	-61
4	120	-140
-1	43*	24
-2	42*	0
-3	43*	-70
-4	80	115
-5	46*	-54
-6	188	177
-7	71	60
8,6,L		
0	42*	-68
1	85	115
2	83	121
3	142	-152
4	47*	-53
-1	43*	-43
-2	67	-74
-3	66	66
-4	69	-62
-5	143	131
-6	146	-134
8,7,L		
0	211	214
1	43*	-40
2	112	132
3	139	123
4	129	146
-1	44*	9
-2	247	244
-3	44*	71
-4	45*	-41
-5	164	-170
-6	45*	-30
8,8,L		
0	45*	58
1	45*	39
2	206	-201
3	108	-117
-1	106	-63
-2	192	200
-3	67	36
-4	91	-71
-5	88	-56
-6	165	153
8,9,L		
0	160	-150
1	47*	75
2	118	-157
3	107	-131
-1	63	-44
-2	46*	15
-3	122	-102
-4	238	-223
-5	48*	93
8,10,L		
0	44*	-37
1	99	84
2	46*	-30
3	165	185
-1	45*	12
-2	45*	-30
-3	185	175
-4	73	67
-5	157	-159
8,11,L		
0	214	-190
1	67	-77
2	47*	-7
-1	46*	34
-2	130	105
-3	47*	-38
-4	75	-62
8,12,L		
0	72	-24
1	94	94
-1	187	-185
-2	50*	131
-3	143	111
-4	148	121
8,13,L		
0	127	-117
-1	49*	61
-2	164	173
9,1,L		
0	244	208
1	92	83
2	47*	-37
-1	145	-129
-2	233	-230
-3	47*	48
-4	46*	-20
9,2,L		
0	108	70
1	47*	-42
-1	47*	39
-2	47*	-27
-3	130	-116
-4	49*	-66
9,3,L		
0	72	30
1	49*	46
-1	47*	14
-2	46*	15
-3	51*	-86
-4	90	83
9,4,L		
0	235	189
1	48*	11
-1	85	56
-2	117	136
-3	66	9
-4	101	-94
9,5,L		
0	139	-110
1	193	170
-1	48*	-34
-2	47*	-52
-3	75	84
9,6,L		
0	178	194
-1	132	111
-2	107	-52
-3	100	-105
9,7,L		
-1	101	-103
-2	193	207

$E_{4,14,\bar{4}}$ which was judged positive with an associated probability of 0·974. Despite this strong indication, the positive sign proved false. By fixing $E_{4,14,\bar{4}}$ as negative through one cycle of Σ_2 and repeating the sign determining procedure a set of signs was produced which yielded an E map which clearly indicated the structure. Of the 209 measured reflections with $|E_{hkl}| \geq 1{\cdot}8$, 207 met the criterion of $p \geq 0{\cdot}989$. These were assigned phases accordingly and all proved to be correct. The remaining two phases had associated probabilities of 0·822 and 0·985 and these proved correct as well.

The structure was refined on F_{hkl}'s by a full-matrix least-squares analysis. The complete data were included in this procedure (2091 observed and 894 unobserved reflections). Reflections were given unit weight for scaled $F_o \leq 20$; reflections with scaled $F_o > 20$ received the weight 20/(scaled F_o). Sixty-nine positional parameters, twenty-three isotropic temperature factors and a scale constant were varied. The refinement was terminated when both R and $\Sigma w(F_o - F_c)^2$ ceased to change significantly. The largest value of the ratio of shift to standard deviation, for any parameter, was 0·0033. At this time R had a value of 0·089. The final values of the parameters are listed in Table 1. The final observed and calculated structure factors are given in Table 2.

Atomic scattering factors used were for O^-, B and Na^+ (*International Tables for X-ray Crystallography*, 1962).

Discussion of the structure

It is of interest to describe this structure by comparing it with previously reported borate structures. Crystalline $Na_2O.4B_2O_3$ resembles, in some characteristic respects, $Ag_2O.4B_2O_3$ (Krogh-Moe, 1965) and $BaO.2B_2O_3$ (Block & Perloff, 1965). All three compounds consist of six-membered rings of alternating boron and oxygen atoms. Some of the rings share a tetrahedral boron atom and thus form double rings, to the extent that single and double rings exist in equal number. Additional oxygen atoms are bonded to the boron atoms so that each boron atom has either a triangular or tetrahedral configuration of neighboring oxygen. These non-ring oxygen atoms also serve as bridges between rings. In this manner three-dimensional networks are formed.

Both $Na_2O.4B_2O_3$ and $Ag_2O.4B_2O_3$ have a ratio of triangular to tetrahedral boron of 3:1. A 1:1 ratio is found in $BaO.2B_2O_3$. Both the sodium and silver compounds consist of two symmetry-related independent networks whereas the barium compound exists as a

Table 3. *Boron–oxygen bond lengths and angles*

Triangularly coordinated boron:

Distances		$\sigma \times 10^3$	Angles		σ
B(1)-O(1)	1·352 Å	6 Å	O(1)—B(1)-O(2)	113·66°	0·37°
O(2)	1·391	6	O(1)—B(1)-O(5)	126·46	0·40
O(5)	1·356	6	O(2)—B(1)-O(5)	119·81	0·39
B(2)-O(2)	1·375	6	O(2)—B(2)-O(3)	122·26	0·40
O(3)	1·353	6	O(2)—B(2)-O(4)	119·65	0·40
O(4)	1·367	6	O(3)—B(2)-O(4)	118·02	0·41
B(4)-O(6)	1·331	6	O(6)—B(4)-O(7)	122·15	0·40
O(7)	1·390	6	O(6)—B(4)-O(10)	119·37	0·39
O(10)	1·375	6	O(7)—B(4)-O(10)	118·46	0·40
B(5)-O(7)	1·379	6	O(7)—B(5)-O(8)	112·93	0·36
O(8)	1·383	6	O(7)—B(5)-O(9)	121·87	0·38
O(9)	1·338	6	O(8)—B(5)-O(9)	125·20	0·38
B(6)-O(10)	1·369	6	O(10)-B(6)-O(11)	110·89	0·37
O(11)	1·396	6	O(10)-B(6)-O(13)	126·62	0·39
O(13)	1·340	6	O(11)-B(6)-O(13)	122·48	0·39
B(7)-O(8′)	1·377	6	O(8′)-B(7)-O(11)	118·93	0·37
O(11)	1·387	6	O(8′)-B(7)-O(12)	119·53	0·39
O(12)	1·341	5	O(11)-B(7)-O(12)	121·25	0·39
Average	1·367			119·97	

Tetrahedrally coordinated boron

Distances		$\sigma \times 10^3$	Angles		σ
B(3)-O(4)	1·448 Å	6 Å	O(4)—B(3)-O(5)°	113·91	0·35°
O(5)	1·462	6	O(4)—B(3)-O(6)	110·39	0·35
O(6)	1·465	5	O(4)—B(3)-O(9)	109·50	0·32
O(9)	1·511	5	O(5)—B(3)-O(6)	106·63	0·32
			O(5)—B(3)-O(9)	106·51	0·34
			O(6)—B(3)-O(9)	109·77	0·33
B(8)-O(1′)	1·461	5	O(1′)-B(8)-O(3′)	111·85	0·34
O(3′)	1·453	5	O(1′)-B(8)-O(12)	107·31	0·31
O(12)	1·490	6	O(1′)-B(8)-O(13)	106·52	0·33
O(13)	1·491	5	O(3′)-B(8)-O(12)	113·23	0·34
			O(3′)-B(8)-O(13)	108·18	0·31
			O(12)-B(8)-O(13)	109·53	0·33
Average	1·473			109·44	

single network. The two networks of $Na_2O.4B_2O_3$ are shown in Fig. 1, projected down the [100] direction. $Na_2O.4B_2O_3$ and $BaO.2B_2O_3$ are also similar in that in each of these compounds single rings are linked only to double rings, double rings being linked only to single rings. (These two structures are compared in Fig. 2.) This ring sequence is not followed, however, in the silver compound. There, single and double rings are each linked to two single and two double rings. One half of a double ring is linked to single rings, the other half to double rings.

The cations in $Na_2O.4B_2O_3$ appear in two crystallographically different environments. They apparently serve to hold the two independent networks together. Na(1) has eight nearest neighbor oxygen atoms; Na(2) has seven. The Na–O distances, which are listed in Table 4, show a considerable variation, ranging from 2·259 to 2·926 Å, with a mean distance of 2·563 Å. B–O bond distances and O–B–O angles are listed in Table 3. The B–O distances are fairly regular with mean values for triangular and tetrahedral boron atoms being respectively 1·367 and 1·473 Å. The mean O–B–O angles are 119·97 and 109·44° respectively for the triangular and tetrahedral boron atoms. These distances and angles are in agreement with those found in other borates.

Table 4. *Sodium–oxygen distances**

Na(1)–O(1)	2·475 Å	Na(2)–O(3)	2·887 Å
O(2)	2·259	O(4)	2·443
O(5)	2·732	O(5)	2·503
O(8)	2·926	O(6)	2·589
O(9)	2·331	O(7)	2·520
O(10)	2·751	O(8)	2·655
O(11)	2·403	O(13)	2·519
O(12)	2·625		
Average	2·563		2·588

* All standard deviations from these distances have a value of 0·004 Å.

Boron coordination

The determination of the relative numbers of triangularly and tetrahedrally coordinated boron atoms as a function of composition has been discussed previously by Edwards & Ross (1960), Krogh-Moe (1962) and by Block & Piermarini (1964). It has been observed in all the borates of known structure that boron atoms are in either three- or four-fold coordination with respect to oxygen. Likewise it is seen that in most of the borates with more than 50 mole% B_2O_3, each oxygen atom is linked to two boron atoms. Under these conditions the ratio of triangular to tetrahedral boron is determined by the stoichiometry. To each triangular boron atom, 3/2 oxygen atoms may be assigned uniquely, two oxygen atoms being assigned uniquely to each tetrahedral boron. The ratio of oxygen to boron may be written as: $(\frac{3}{2}N_3+2N_4)/(N_3+N_4)$, where N_3 and N_4 are respectively the numbers of triangular and tetrahedral boron atoms per some arbitrary amount of compound. If the stoichiometric formula of a borate is written as $M_xO.nB_2O_3$, the oxygen to boron ratio is given by $(3n+1)/2n$. Equating these expressions and rearranging yields for the triangular to tetrahedral boron ratio: $N_3/N_4=n-1$. Krogh-Moe (1962) obtained this result by considering a particular reaction scheme between an oxide and a borate network. The rule will

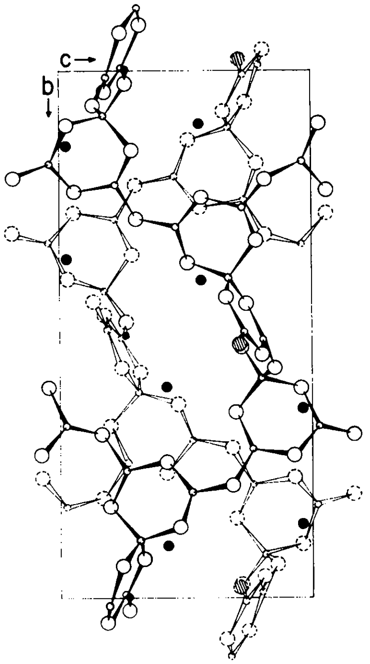

Fig. 1. The two networks of $Na_2O.4B_2O_3$, projected along **a**. The large open circles represent oxygen atoms. The small open circles represent boron atoms. One network is indicated by dashed circles and open links, the other by unbroken circles and filled links. The solid circles represent sodium atoms. The shaded circles represent atoms from the next unit cell along **a**. These have been displaced slightly for clarity.

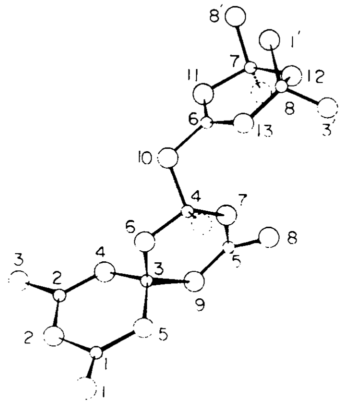

Fig. 2. Diagrammatic comparison of the boron–oxygen networks of $Na_2O.4B_2O_3$ and $BaO.2B_2O_3$. The large and small circles represent respectively oxygen and boron atoms. The dotted circles belong only to the Ba compound. All other circles are common to both structures. The numbering used in the figure is consistent with that used in Table 1.

Table 5. *The ratio of triangular to tetrahedral boron as a function of volume/atom*

Compound	Reference	Volume/atom	Ratio of triangular to tetrahedral boron
$PbO.2B_2O_3$	Perloff & Block (1966)	13·406	0
$SrO.2B_2O_3$	Perloff & Block (1966) Krogh-Moe (1964)	12·482	0
$BaO.2B_2O_3$	Block & Perloff (1965)	17·227	1
$CdO.2B_2O_3$	Ihara & Krogh-Moe (1966)	17·266	1
$Li_2O.2B_2O_3$	Krogh-Moe (1962)	16·070	1
$Cs_2O.3B_2O_3$	Krogh-Moe (1960)	17·775	2
$Ag_2O.4B_2O_3$	Krogh-Moe (1965)	17·197	3
$Na_2O.4B_2O_3$	This paper	17·780	3
$K_2O.5B_2O_3$	Krogh-Moe (1959)	18·019	4
$Rb_2O.5B_2O_3$	Krogh-Moe (1959)	17·893	4

* The volume/atom is calculated as $V/[N_O+N_c(r_c/1\cdot4)^3]$, where V is the volume per unit mass, N_O and N_c are respectively the number of oxygen atoms and cations per unit mass, and r_c is the radius of the cation in Å. The term $(r_c/1\cdot4)^3$ accounts for the volume occupied by a cation relative to that occupied by an oxygen atom.

hold for hydrated borates as well, provided that water enters the structure *via* the scheme:

$$H_2O+BOB\rightarrow 2B\text{–}OH.$$

The rule will not hold in the event of some unusual coordination, such as is found in $SrO.2B_2O_3$, where some of the oxygen is coordinated to three boron atoms.

It may be useful to establish techniques for determining *a priori* whether or not such unusual bonding exists. In this connection it is observed that in borates with more than 50 mole% B_2O_3, calculated values of the volume per atom (excluding boron) indicate the presence or absence of unusual coordination. Table 5 lists the volume per atom for a number of anhydrous borates. $SrO.2B_2O_3$ and its isomorph $PbO.2B_2O_3$ have values of this quantity less than 14 Å^3, whereas in all other compounds the volume per atom lies between 16 Å^3 and 19 Å^3. Thus on the basis of density measurements the existence of unusual coordination may be inferred.

With the exceptions of a program which edits the paper tape output of the diffractometer, and a Σ_2 sign generating program, computations were made with the aid of programs incorporated into the X-ray 63 system developed at the University of Maryland Computer Science Center (1964) and the University of Washington. The paper tape editing program has since been made a part of the system.

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