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The Crystal Structure of the Basic Mercury(II) Perchlorate $Hg_2OOHClO_4$

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The crystal structure of $Hg_2OOHClO_4$ has been determined from three-dimensional X-ray data using visually estimated intensities from Weissenberg photographs. The unit cell is monoclinic with $a = 11.078$ Å, $b = 14.269$ Å, $c = 7.224$ Å, and $\beta = 100.5°$. The space group is No. 14: $P2_1/c$. Each Hg atom forms two short Hg–O bonds with lengths of 2.0 Å and with the O–Hg–O angle close to 180°. Other Hg–O contacts are longer than about 2.7 Å. The structure can be described as built up from infinite one-dimensional complexes in which the Hg atoms are joined by the covalently bonded oxygens. The characteristic OHg_3 groups, previously found in several other structures, can be distinguished in these complexes.

In connection with an X-ray investigation of the structures of the polynuclear hydrolysis complexes of mercury(II) in aqueous perchlorate solutions,[1] it was found of interest to determine the structures of the basic salts that could be crystallized from such solutions. Of particular interest is the coordination of the mercury atom in the crystals and the type of bridging between the metal atoms in the polynuclear complexes. The structure of the basic perchlorate $Hg_5O_2(OH)_2(ClO_4)_4(H_2O)_x$, which is the least basic of those obtained, has been described in a previous paper.[2] The crystal structure of the most basic of the salts, $Hg_2OOHClO_4$, is given in the present paper, and an intermediate phase, $Hg_7O_4(OH)_2(ClO_4)_4$, will be discussed in a following paper.

EXPERIMENTAL

Preparation of crystals. Solutions obtained by dissolving an excess of HgO in $HClO_4$ were used for the preparation of the crystals. Needlelike or rod-shaped crystals suitable for X-ray work crystallize spontaneously from a solution which is 3.1 M in Hg^{2+} and 4.8 M in ClO_4^-. The crystals are stable outside the mother liquor but decompose to HgO when washed with water.

Analysis. The crystals were separated from the mother liquor by centrifuging and were dried between filter papers. Dilute perchloric acid was used to dissolve the crystals before analysis.

Mercury was determined by reducing with H_3PO_3 and precipitating and weighing as Hg_2Cl_2. Perchlorate was determined by passing a portion of a solution through a cation exchanger and titrating the eluate with NaOH, correcting for the amount of $HClO_4$ used to dissolve the crystals. The density was calculated from the apparent loss of weight in benzene.

The results of the analysis are compared in Table 1 with values calculated for the stoichiometric composition $4HgO \cdot Cl_2O_7 \cdot H_2O$. A basic mercury(II) perchlorate, probably identical with the one described here, has been prepared previously by Hayek and Schnell.[3] They assumed the composition to be $4HgO \cdot Cl_2O_7$ and the results of their analysis are given in Table 1 for comparison.

Table 1. Analytical data.

	Found	Calculated for $4\,HgO.Cl_2O_7.H_2O$	Found by Hayek and Schnell [3]
% HgO	79.0	81.3	81.3
% Cl_2O_7	18.2	17.1	18.1
% H_2O	2.8 (diff.)	1.7	
Density (g cm^{-3})	6.1_3	6.28	

For a direct estimation of the number of non-perchlorate oxygens a Karl Fischer titration [4] was carried out. It can be expected that basic oxygens (O^{2-} and OH^-) will react as water in this titration and the result will give the total number of oxygens not belonging to the perchlorate groups. Eight different titrations gave an average value of 0.9_4 such oxygens per mercury atom. It will be shown in the folllowing, that the crystal structure determination indicates that the correct formula is $Hg_2OOHClO_4$. This is consistent with the number of oxygens estimated from the Karl Fischer titration and corresponds to the stoichiometric composition $4HgO \cdot Cl_2O_7 \cdot H_2O$.

Unit cell and space group. Weissenberg photographs taken along two of the axes of the unit cell showed the symmetry to be monoclinic. More accurate values for the unit cell dimensions than those obtained from the Weissenberg photographs were determined by a least squares refinement using the line positions on a powder photograph taken in a Guinier camera. Cu$K\alpha$ radiation ($\lambda = 1.5405$ Å) was used with KCl ($a = 6.2929$ Å) as internal standard. Observed and calculated line positions for the first part of the powder photograph are given in Table 2. The unit cell dimensions were found to be:

$$a = 11.07_8 \text{ Å},\ b = 14.26_9 \text{ Å},\ c = 7.22_4 \text{ Å},\ \beta = 100.5°$$

The calculated density, assuming four formula weights $4HgO.Cl_2O_7.H_2O$ in the unit cell, is 6.28. The observed value is 6.1_3 (Table 1). Systematically absent reflections are $h0l$ for $l = 2n+1$ and $0k0$ for $k = 2n+1$. This is consistent with the centrosymmetric space group No. 14, $P2_1/c$.

Intensity data. Intensity data were collected in a Weissenberg camera with the use of Mo$K\alpha$ radiation. Crystals with as far as possible cylindrical cross sections, with the largest dimension not exceeding 0.10 mm, were selected. Photographs were taken around the c axis ($hk0 - hk8$) and the b axis ($h0l - h4l$). Intensities were determined by visual comparison with an intensity scale prepared by timed exposures of one of the reflections of the same crystal. Intensities for about 2350 independent reflections were determined and were used for the structure determination. Lorentz and polarization factors were applied in the usual way and all intensities were recalculated to a common scale with the use of reflections appearing on more than one photograph.

Computer programs. The following programs were used to carry out the calculations:

DRF. Lp corrections, structure factor calculations and Fourier summations. Originally written by A. Zalkin, Berkeley, USA. Modified by R. Liminga and J. O. Lundgren, Uppsala, Sweden.

Table 2. Calculated and observed $\sin^2\theta$ values for the first lines of a Guinier powder photograph of $Hg_2OOHClO_4$.

hkl	$(\sin^2\theta)_{calc}$	$(\sin^2\theta)_{obs}$	I_{obs}
110	0.00792	0.00789	vvw
020	0.01166	0.01165	vw
011	0.01467	0.01465	m
11$\bar{1}$	0.01680	0.01677	s
200	0.02000	0.01998	w
111	0.02255	0.02251	m
210	0.02292	0.02290	vvw
021	0.02341	0.02342	vw
121	0.03129	0.03126	w
220	0.03166	0.03163	w
22$\bar{1}$	0.03767	0.03766	m
031	0.03799	0.03796	vw
300	0.04501	0.04498	s
310	0.04792	0.04792	vw
221	0.04917	0.04910	vvw
112	0.04920		
012	0.04995	0.04999	m
140	0.05163	0.05163	s
23$\bar{1}$	0.05224	0.05221	vw
202	0.05554	0.05555	vvw
320	0.05666	0.05661	w
102	0.05778	0.05780	s
022	0.05869	0.05873	s
14$\bar{1}$	0.06051	0.06053	w
240	0.06663	0.06663	w
222	0.06719	0.06723	w
311	0.06830	0.06835	w
330	0.07123	0.07122	vw
24$\bar{1}$	0.07264	0.07262	vw
33$\bar{1}$	0.07437	0.07444	w
150	0.07785	0.07781	vs
312	0.07771		
400	0.08001	0.08013	vvw
232	0.08177	0.08179	m
41$\bar{1}$	0.08319	0.08299	vw
132	0.08401	0.08416	s
241	0.08414		
322	0.08645	0.08646	w
222	0.09019	0.09013	vvw
420	0.09167	0.09170	vw
42$\bar{1}$	0.09193		
250	0.09286	0.09279	vw
042	0.09366	0.09362	vvw
34$\bar{1}$	0.09477	0.09482	vvw
251	0.09887	0.09891	w
232	0.10476	0.10489	vw
060	0.10491		
113	0.10512		

LALS. Full matrix least squares refinement. Originally written by P. K. Gantzel, R. A. Sparks and K. N. Trueblood, Los Angeles, USA. Modified by A. Zalkin, Berkeley, USA, and by J.-O. Lundgren, R. Liminga and C. I. Brändén, Uppsala, Sweden.

DISTAN. Calculations of interatomic distances and bond angles. Written by A. Zalkin, Berkeley, USA, and modified by A. G. Nord and B. G. Brandt, Stockholm, Sweden.

STRUCTURE DETERMINATION

The three-dimensional Patterson function showed that the 16 Hg atoms in the unit cell must occupy the general four-fold positions. Possible parameter values were deduced from the Harker sections. A systematic comparison of calculated Hg – Hg vectors with peaks in the three-dimensional Patterson function, sufficiently high to be identified as possible Hg – Hg vectors, led to an apparently unique set of parameter values for the four four-fold Hg positions in the unit cell.

A least squares refinement of the derived positions using all observed reflections gave an R factor of 0.20 and led to reasonable temperature factors for the four independent Hg atoms. On the basis of the derived parameter values a three-dimensional difference map was calculated from which the chlorine atoms and most of the oxygen atoms could be located. A new least squares refinement followed by a three-dimensional difference map led to the positions of the remaining oxygen atoms.

With all atoms included, a new least squares refinement using all observed reflections and with individual isotropic temperature factors for all atoms lowered the R factor to 0.16. The scattering factors used were those given by Cromer and Waber [5] for the neutral atoms. Corrections were made for the real part of the anomalous dispersion according to Cromer.[6] The weighting scheme was that suggested by Hughes.[7] A further least squares refinement

Table 3. Final parameters for $Hg_2OOHClO_4$. All atoms are in position 4(*e*) in space group No. 14; $P2_1/c$. Standard deviations are given within brackets.

Atom	x	y	z	B
Hg_1	0.3207 (2)	0.2484 (1)	0.9784 (2)	1.1 (0)
Hg_2	0.2649 (2)	0.0487 (1)	0.2020 (2)	1.2 (0)
Hg_3	0.6744 (2)	0.1842 (1)	0.9093 (2)	1.5 (0)
Hg_4	0.9654 (2)	0.1114 (1)	0.8376 (2)	1.5 (0)
Cl_1	0.9604 (10)	0.1384 (8)	0.3462 (15)	1.7 (2)
O_1	0.0179 (54)	0.0951 (44)	0.2192 (83)	4.5 (14)
O_2	0.8802 (44)	0.1973 (38)	0.2621 (68)	2.7 (8)
O_3	0.8921 (47)	0.0891 (40)	0.4314 (73)	4.1 (12)
O_4	0.0495 (49)	0.1865 (40)	0.4756 (73)	3.1 (10)
Cl_2	0.3999 (11)	0.4777 (9)	0.2354 (15)	1.8 (2)
O_5	0.3056 (36)	0.4359 (30)	0.1011 (53)	1.6 (7)
O_6	0.5195 (63)	0.4575 (53)	0.2045 (97)	4.5 (15)
O_7	0.6071 (56)	0.0779 (50)	0.2629 (84)	4.5 (15)
O_8	0.4032 (74)	0.4336 (63)	0.4399 (114)	5.8 (19)
O_9	0.7805 (27)	0.4141 (22)	0.3069 (39)	1.9 (6)
O_{10}	0.3341 (30)	0.1834 (23)	0.2254 (43)	1.7 (6)
O_{11}	0.5754 (37)	0.2685 (30)	0.0350 (54)	3.1 (10)
O_{12}	0.1422 (36)	0.3822 (29)	0.3815 (54)	2.9 (9)

Table 4. Observed and calculated structure factors.

0 k 0		5 k 0		14 74 - 74		13 180 -184		14 61 - 59		3 61 - 76		16 99 - 95	
0 1800		0 254 -255		15 < 52 10		14 85 80		15 < 41 - 23		4 108 140		17 < 48 22	
2 125 -119		1 62 93		16 130 102		15 51 - 50		16 109 -123		5 211 278		18 < 50 - 29	
4 98 31		2 199 241		17 < 55 38		16 < 42 9		17 104 108		6 76 75		19 149 174	
6 288 -259		3 52 - 34		18 120 -115		17 121 142		18 52 46		7 50 - 40		9 k	
8 73 - 21		4 229 -247		10 k 0		18 127 134		19 < 48 - 26		8 < 34 - 7		1 119 -144	
10 167 -131		5 63 - 75		0 100 - 95		19 < 45 - 33		20 < 50 43		9 143 -177		2 49 57	
12 < 40 - 18		6 < 32 17		1 112 107		20 < 49 41		21 114 142		10 36 39		3 127 -154	
14 378 -433		7 442 -524		2 57 - 50		21 57 66		-3 k 1		11 37 36		4 < 37 36	
16 265 284		8 127 133		3 189 203		1 k 1		1 90 - 82		12 < 39 26		5 167 198	
18 < 50 - 11		9 165 174		4 88 95		1 232 -253		2 108 -112		13 < 40 - 29		6 56 38	
20 136 157		10 170 188		5 98 - 92		2 152 200		3 455 -392		14 106 -133		7 < 38 21	
		11 55 42		6 < 43 8		3 112 85		4 278 207		15 < 44 21		8 < 39 1	
1 k 0		12 92 - 97		7 183 157		4 150 -105		5 < 27 - 30		16 151 -181		9 62 - 67	
0 < 12 9		13 127 125		8 < 45 19		5 295 -257		6 66 71		17 < 47 28		10 < 39 7	
1 60 - 65		14 125 145		9 143 -117		6 197 -175		7 63 46		18 < 54 - 28		11 142 135	
2 191 139		15 < 47 41		10 < 47 3		7 213 179		8 130 107		19 89 -105		12 < 43 - 28	
3 < 14 - 10		16 167 -161		11 172 136		8 149 -136		9 258 236		-6 k 1		13 70 56	
4 473 499		17 < 50 53		12 110 88		9 366 343		10 63 54		1 41 40		14 < 46 - 37	
5 625 597		18 82 89		13 < 51 - 53		10 74 - 44		11 251 264		2 116 -109		15 < 47 51	
6 87 - 74		19 < 54 18		14 < 52 29		11 < 33 12		12 175 -167		3 338 -330		16 < 49 - 61	
7 130 109		20 79 - 85		15 119 - 97		12 238 -227		13 89 - 96		4 44 30		17 < 50 - 29	
8 179 195		21 81 104		16 < 55 - 10		13 165 152		14 < 39 - 17		5 68 - 64		18 < 52 - 12	
9 422 -416		22 < 60 - 51		17 113 - 78		14 71 - 74		15 63 - 63		6 201 -195		19 129 -142	
10 167 190		23 109 -132				15 < 40 - 14		16 < 42 - 13		7 < 31 19			
11 227 239				11 k 0		16 91 - 89		17 111 112		8 121 -118		-9 k 1	
12 139 -160		6 k 0		0 241 -215		17 101 - 91		18 100 - 98		9 229 218		1 171 162	
13 49 57		0 184 209		1 54 38		18 < 45 40		19 85 - 90		10 122 117		2 76 - 64	
14 < 42 26		1 157 190		2 221 181		19 < 47 13		4 k 1		11 211 215		3 61 - 54	
15 127 134		2 348 -422		3 116 100		20 75 54		1 102 -150		12 < 38 13		4 < 35 22	
16 77 - 77		3 155 208		4 < 44 28		21 148 -161		2 131 181		13 79 - 84		5 < 35 8	
17 72 50		4 < 32 6		5 < 44 41		-1 k 1		3 149 174		14 133 130		6 244 -207	
18 126 135		5 87 97		6 < 45 15		1 - 310		4 212 -257		15 48 - 52		7 < 37 - 35	
19 132 136		6 < 34 8		7 107 - 80		2 < 14 5		5 101 -112		16 49 55		8 180 -139	
20 < 54 - 14		7 208 -227		8 129 -106		3 79 51		6 194 -218		17 86 90		9 < 39 13	
21 124 -138		8 111 108		9 < 48 49		4 421 -365		7 < 29 17		18 < 48 - 4		10 145 126	
22 < 57 - 50		9 125 145		10 109 - 74		5 174 -127		8 226 -225		19 79 - 69		11 < 41 21	
23 < 59 70		10 90 94		11 < 50 16		6 261 225		9 45 54				12 < 43 47	
24 < 61 - 27		11 < 41 14		12 117 - 98		7 143 -107		10 < 36 - 66		7 k 1		13 115 -101	
25 133 -161		12 209 203		13 < 53 - 30		8 154 130		11 120 122		1 < 30 38		14 110 104	
		13 < 44 - 9		14 126 113		9 68 - 48		12 243 267		2 106 147		15 < 47 - 31	
2 k 0		14 155 -175		15 < 55 - 49		10 258 -224		13 162 146		3 162 212		16 < 48 19	
0 218 -236		15 125 -147		16 102 - 94		11 101 -101		14 < 40 15		4 91 -123		17 89 76	
1 120 141		16 159 172		17 < 58 - 50		12 121 114		15 < 42 15		5 < 31 - 5		18 < 51 9	
2 101 102		17 81 - 63		18 84 73		13 217 -204		16 < 43 0		6 < 33 - 44		19 < 53 4	
3 49 56		18 127 -135				14 < 37 11		17 48 - 74		7 48 - 39		20 96 87	
4 417 -449		19 < 55 - 23		12 k 0		15 56 - 54		18 81 103		8 49 - 50			
5 337 302		20 < 57 - 20		0 71 55		16 110 108				9 175 -163		10 k 1	
6 < 27 26		21 82 84		1 < 45 29		17 103 104		-4 k 1		10 64 - 48		1 37 - 50	
7 357 -328				2 78 - 71		18 134 134		1 327 328		11 189 -225		2 105 114	
8 322 312		7 k 0		3 64 - 55		19 107 -109		2 255 240		12 132 156		3 110 129	
9 314 299		0 90 106		4 181 131				3 53 - 35		13 63 73		4 < 38 3	
10 317 332		1 114 130		5 < 45 - 3		2 k 1		4 46 - 44		14 57 - 39		5 58 55	
11 87 - 82		2 80 102		6 < 48 38		1 65 - 83		5 117 -108		15 < 45 31		6 109 135	
12 66 - 72		3 329 359		7 200 -171		2 84 113		6 358 298		16 < 46 - 33		7 < 40 - 15	
13 63 56		4 41 45		8 117 -103		3 72 - 76		7 73 - 59		17 < 48 - 32		8 81 89	
14 119 119		5 157 -160		9 90 72		4 437 495		8 203 168		18 74 67		9 97 -100	
15 58 - 48		6 56 - 63		10 95 - 65		5 58 - 51		9 48 48		19 91 71		10 57 - 52	
16 149 -148		7 260 240		11 < 52 4		6 < 27 - 4		10 129 -116				11 121 -127	
17 < 48 0		8 < 47 - 16		12 < 53 50		7 < 28 28		11 < 35 3		1 80 91		12 50 77	
18 79 79		9 134 -127		13 77 70		8 < 28 - 13		12 85 79		2 339 274		13 83 72	
19 82 - 69		10 90 - 88				9 < 30 25		13 213 -215		3 194 -172		14 80 - 79	
20 96 -124		11 198 237		13 k 0		10 269 273		14 163 -154		4 < 30 28			
21 125 136		12 90 - 75		0 116 -105		11 < 33 25		15 73 - 71		5 58 - 50		-10 k 1	
22 93 -106		13 79 - 80		1 < 48 17		12 104 - 98		16 94 - 92		6 160 156		1 67 - 42	
		14 < 47 - 21		2 114 - 78		13 51 - 59		17 98 109		7 33 53		2 134 128	
3 k 0		15 133 -130		3 < 49 20		14 89 - 87		18 < 46 19		8 < 34 33		3 161 -154	
0 610 851		16 < 51 0		4 87 77		15 < 40 22		19 102 90		9 169 165		4 100 - 91	
1 185 244		17 125 -115		5 163 -114		16 208 -211				10 100 - 95		5 < 38 8	
2 274 -321		18 < 54 46		6 < 50 17		17 < 44 - 6		5 k 1		11 173 155		6 175 - 70	
3 217 246		19 < 56 82		7 < 51 60		18 148 -144		1 202 -270		12 115 119		7 < 39 38	
4 64 33		20 < 58 45		8 < 52 7		19 < 47 25		2 98 48		13 91 - 97		8 85 - 79	
5 241 217		21 < 59 - 54		9 132 -100		20 124 124		3 32 - 35		14 155 -146		9 99 97	
6 128 -108		22 < 61 16		10 < 53 0				4 191 251		15 < 44 - 36		10 45 - 48	
7 59 - 61		23 138 124		11 85 64		-2 k 1		5 < 28 27		16 120 -133		11 154 135	
8 62 64				12 119 92		1 < 30 - 27		6 145 -166				12 164 156	
9 145 129		8 k 0				2 343 -303		7 99 105		8 k 1		13 < 46 - 5	
10 56 - 38		0 155 -162		14 k 0		3 275 221		8 86 - 89		1 107 -110		14 53 - 44	
11 45 - 20		1 < 35 40		0 255 194		4 261 -182		9 49 48		2 99 -124			
12 103 89		2 294 309		1 < 51 - 4		5 543 -489		10 186 204		3 51 67		11 k 1	
13 109 - 95		3 < 46 10		2 71 54		6 201 -143		11 109 106		4 < 33 23		1 39 - 5	
14 316 -337		4 51 - 54		3 72 54		7 163 119		12 < 38 5		5 53 70		2 107 -112	
15 214 -198		5 87 - 91		4 < 51 - 12		8 139 -109		13 153 141		6 197 -215		3 116 118	
16 246 247		6 < 38 8		5 89 59		9 362 305		14 < 41 25		7 44 42		4 < 40 - 4	
17 136 -117		7 296 -332		6 < 53 17		10 < 31 - 17		15 64 65		8 90 - 90		5 64 58	
18 71 - 65		8 92 - 90		7 < 53 27		11 < 33 - 25				9 60 - 44		6 91 - 90	
20 77 85		9 84 83		8 < 54 - 25		12 101 - 88		-5 k 1		10 93 108		7 < 42 - 23	
21 79 68		10 < 43 - 36		9 < 55 30		13 57 48		1 270 273		11 < 41 - 8		8 < 42 - 29	
		11 < 44 43				14 187 180		2 109 -101		12 < 42 2		9 97 -114	
4 k 0		12 164 -163		15 k 0		15 66 - 53		3 233 225		13 121 118		10 50 32	
00 173 189		13 66 49		0 < 53 47		16 173 167		4 77 - 71		14 83 99		11 85 - 93	
1 < 32 39		14 119 120		1 < 53 - 1		17 46 - 46		5 445 -393		15 77 58		12 66 - 64	
2 242 281		15 < 51 3		2 < 53 - 2		18 63 44		6 225 -181		16 67 68		13 54 41	
3 215 256		16 110 -122		3 < 53 - 24		19 87 102		7 57 - 44		17 78 - 92		14 56 50	
4 133 -139		17 < 54 7		4 93 84		20 < 49 - 24		8 142 -125					
5 438 -468		18 87 116		5 75 64		21 128 -145		9 105 115		-8 k 1		-11 k 1	
6 125 -130				6 < 55 34				10 < 34 7		1 109 103		1 71 - 58	
7 161 153		9 k 0		7 < 56 - 48		3 k 1		11 188 -178		2 109 112		2 176 151	
8 < 36 - 18		0 59 48		8 79 - 87		1 313 380		12 < 37 5		3 163 149		3 82 66	
9 276 -265		1 75 84				2 126 170		13 86 - 87		4 125 120		4 150 137	
10 93 - 94		2 278 -275		0 k 1		3 < 24 - 27		14 70 77		5 251 -230		5 140 -116	
11 290 310		3 < 64 1		1 - 253		4 65 - 55		15 55 - 61		6 < 34 9		6 < 40 34	
12 211 -203		4 89 81		2 - 137		5 197 219		16 49 53		7 < 35 - 22		7 44 47	
13 < 42 0		5 < 40 - 23		3 271 -207		6 75 - 70		17 < 45 28		8 36 - 41		8 < 42 - 7	
14 43 - 41		6 < 41 24		4 261 -189		7 180 -162		18 < 47 33		9 37 48		9 93 74	
15 < 45 - 1		7 311 -257		5 72 47		8 88 - 86		19 216 210		10 41 38		10 81 58	
16 < 47 - 20		8 < 43 - 12		6 337 -249		9 220 -240				11 188 -184		11 63 - 57	
17 < 49 - 28		9 106 99		7 90 - 69		10 60 49		6 k 1		12 < 41 20		12 < 46 40	
18 143 150		10 < 45 42		8 231 -195		11 < 34 - 24		1 33 40		13 62 - 57		13 < 47 47	
19 130 137		11 < 46 36		9 29 - 26		12 177 142		2 215 252		14 60 - 56		14 87 - 69	
20 88 88		12 179 170		10 45 37		13 160 -161				15 < 45 - 33		15 < 50 1	
21 80 - 90		13 75 92		11 103 98									
				12 293 284									

Table 4. Continued.

16	113	-109	3	196	192	10	< 90	76	6	< 97	36	7	71	- 60	12	127	-153	14	134	-121
	12 k 1		4	85	60	11	< 94	-105	7	156	130	8	146	138	13	164	194	15	< 77	12
1	83	- 82	5	244	230	12	< 98	- 30	8	< 101	- 80	9	198	-196	14	< 71	- 33	16	138	-187
2	70	- 61	6	290	282	13	114	-121	9	< 102	26	10	94	84	15	< 74	23		8 k 3	
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2	47	45	4	< 51	- 17	10	106	- 77	8	141	130	2	91	-121	9	< 54	- 36	12	141	-168
3	< 41	20	5	202	-151	11	215	210	9	149	-134	3	168	-174	10	133	126		-8 k 3	
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	13 k 1		8	< 71	- 21	0	164	185	12	< 109	- 50	6	260	-221	13	< 66	34	3	< 54	- 8
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1	87	- 71		-6 k 2		2	< 73	- 44	14	142	-170	8	195	-142	15	< 72	72	5	57	- 57
2	47	45		3 k 2		3	170	-188		10 k 2		9	185	-153	16	125	-110	6	164	-186
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7	< 46	21	4	353	401	8	193	-218	4	93	114	14	151	135	4	92	107	11	92	86
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	-13 k 1		11	< 88	55	3	216	209		-10 k 2		1	111	129	11	< 65	- 18	6	135	149
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3	63	- 64	14	< 101	- 95	6	199	-195	2	52	- 65	4	79	- 85		-5 k 3		9	< 72	- 60
4	87	- 95	15	< 105	- 53	7	218	182	3	< 92	- 20	5	261	269	1	137	-150	10	91	- 84
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	0 k 2		5	234	-273	16	114	120	1	178	-181	14	123	125	10	159	123	8	98	- 97
0	53	- 93	6	119	-101		7 k 2		2	43	42	15	< 72	67	11	91	- 57	9	67	51
1	400	447	7	< 89	76	0	205	-257	3	116	- 99	16	130	131	12	65	71	10	< 69	- 25
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3	< 42	- 6	9	154	-202	2	< 35	26		11 k 2		1	< 23	- 35	14	104	107	12	174	214
4	300	257	10	151	-146	3	47	- 62	0	141	-127	2	149	-116		6 k 3			10 k 3	
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7	251	-187	13	< 108	- 18	6	119	-101	3	< 98	6	5	59	45	3	< 52	9	5	121	-105
8	222	175	14	< 112	114	7	< 89	76	4	170	-197	6	369	286	4	276	-325		-10 k 3	
9	147	-113	15	153	150	8	< 91	55	5	< 100	10	7	122	- 88	5	55	58	1	180	196
10	79	- 61		-7 k 2		9	154	-202	6	< 102	1	8	184	-149	6	69	66	2	96	108
11	169	141	0	125	129	10	151	-146	7	104	15	9	320	-252	7	< 56	- 50	3	62	- 59
12	355	318	1	134	133	11	101	77	8	< 106	140	10	106	82	8	< 61	29	4	< 63	45
13	201	200	2	170	-176	12	< 104	70	9	< 109	- 12	11	325	-270	9	92	- 86	5	< 64	60
14	98	- 81	3	< 40	- 6	13	< 108	- 18	10	152	167	12	< 61	16	10	121	-141	6	< 66	- 25
	4 k 2		4	254	-261	14	< 112	114		12 k 2		13	102	87	11	< 67	- 32	7	74	- 79
15	150	-149	5	221	216	15	153	150	0	< 109	18	14	92	69	12	70	57	8	77	- 63
16	131	144	6	122	97		-8 k 2		1	110	39		3 k 3		13	< 72	17	9	< 71	- 81
17	148	117	7	227	-240	0	125	129	2	112	-107	1	267	-287	14	< 75	77	10	< 73	31
18	201	-197	8	87	56	1	134	133		12 k 2		2	50	37	15	< 78	7	11	< 75	16
	1 k 2		9	239	249	2	170	-176	0	140	134	3	60	- 52	16	90	119	12	< 77	24
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1	< 36	- 7		8 k 2		4	254	-261	2	< 105	- 33	5	69	70	1	128	146		11 k 3	
2	104	125	0	293	-348	5	221	216	3	85	- 98	6	74	84	2	283	280	1	< 71	- 23
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4	138	124	2	< 46	- 29	7	227	-240	0	198	211	8	< 51	0	4	101	- 88	3	120	-106
5	139	-114	3	< 40	- 18	8	87	56	1	105	-102	9	< 55	1	5	< 49	- 19		-11 k 3	
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7	258	211	5	131	151	10	260	268		-14 k 2		11	61	66	7	113	- 92	2	< 65	46
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11	285	262	9	115	111	2	< 46	- 29		-16 k 2		15	< 73	49	11	222	-201	6	< 69	- 16
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13	217	-205		-8 k 2		4	60	- 66	1	< 120	27	17	< 78	- 75	13	< 69	0	8	< 72	21
14	189	207	0	130	-157	5	131	151	2	< 125	- 22	18	129	- 123	14	< 72	- 51	9	112	107
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16	170	-153	2	164	201	7	< 94	- 37		0 k 3		20	139	-117	16	87	- 98		12 k 3	
17	224	-233	3	< 81	35	8	108	-119	1	267	-345		-3 k 3			7 k 3		1	< 71	67
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11	< 83	- 14		9 k 2		9	< 95	- 96	14	149	-147	13	137	109	12	81	- 89	1	117	128
12	138	-142	0	100	97	10	98	116	15	< 70	51	14	180	-176	13	130	139	2	< 72	2
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	2 k 2		2	55	- 69	12	128	-141	17	121	-109	16	217	-220	1	< 49	31	4	84	- 71
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						3	263	301	5	< 48	- 8	7	< 57	4	7	< 59	- 42			
						4	233	241	6	142	175	8	53	69	8	90	- 82			
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Table 4. Continued.

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6	213	-199
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12	129	-115
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15	176	-190
16	< 73	15
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18	88	- 83
19	111	-109
	1 k 4	
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1	510	-502
2	108	130
3	33	35
4	148	151
5	99	-114
6	104	- 96
7	75	71
8	114	-121
9	128	-116
10	201	-191
11	< 58	2
12	75	- 69
13	204	-192
14	< 67	17
15	351	322
16	< 73	- 11
17	101	- 93
18	< 79	36
19	< 82	81
20	95	101
	-1 k 4	
0	510	-439
1	84	- 84
2	133	-161
3	216	-232
4	121	-114
5	217	190
6	421	389
7	117	89
8	391	-302
9	83	70
10	365	291
11	184	-154
12	103	82
13	63	58
14	133	126
15	85	- 67
16	< 72	- 35
17	76	86
18	< 77	- 55
19	108	-102
20	170	-181
21	< 80	- 9
22	101	89
	2 k 4	
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1	89	- 87
2	< 39	- 17
3	278	-326
4	171	-182
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6	313	314
7	< 48	15
8	264	-267
9	< 53	- 22
10	283	269
11	97	- 97
12	< 62	- 21
13	101	124
14	< 68	63
15	133	127
16	< 74	- 23
17	86	164
	-2 k 4	
0	261	-256
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2	< 25	30
3	57	68
4	202	170
5	279	-240
6	63	49
7	86	- 66
8	113	- 91
9	192	-137
10	54	- 37
11	84	67
12	74	53
13	155	-135
14	137	127
15	379	380
	3 k 4	
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1	164	175
2	158	-180
3	232	-263
4	77	90
5	214	214
6	116	-124
7	203	218
8	241	279
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12	151	158
13	< 66	67
14	< 69	- 16
15	135	-152
16	< 75	6
17	< 78	94
18	< 81	- 92
19	94	-118
	-3 k 4	
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1	138	146
2	46	43
3	170	-151
4	421	425
5	< 39	1
6	318	-261
7	138	112
8	< 49	28
9	< 52	- 29
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11	77	- 53
12	95	77
13	128	112
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15	70	- 60
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19	< 82	- 26
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	4 k 4	
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2	67	71
3	143	137
4	146	28
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14	< 71	- 42
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6	340	276
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19	124	-121
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	5 k 4	
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1	150	-140
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3	189	-228
4	162	-173
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6	151	164
7	< 56	27
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9	< 60	- 28
10	113	129
11	< 65	- 79
12	152	-153
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14	< 72	- 32
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17	91	94
	-5 k 4	
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3	299	298
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8	73	- 42
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12	149	113
13	182	-181
14	214	179
15	229	203
16	84	- 85
17	135	-147
18	109	- 99
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	6 k 4	
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2	97	-103
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4	79	- 75
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8	193	210
9	< 63	- 40
10	< 65	49
11	121	-136
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13	135	153
14	< 75	- 25
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16	< 80	12
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	-6 k 4	
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2	123	-115
3	110	-110
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5	269	-221
6	231	-193
7	140	-102
8	142	129
9	104	- 82
10	345	-304
11	92	73
12	155	137
13	146	137
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15	< 74	18
16	< 77	23
17	126	106
18	92	- 91
	7 k 4	
0	55	29
1	193	-214
2	56	- 61
3	134	152
4	< 58	- 47
5	89	95
6	109	-122
7	125	151
8	184	224
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13	124	-143
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2	106	106
3	63	- 41
4	128	117
5	94	76
6	226	185
7	124	-118
8	427	-355
9	74	59
10	83	- 74
11	65	- 50
12	95	- 76
13	111	99
14	< 73	0
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	8 k 4	
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1	56	- 47
2	132	133
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6	94	104
7	< 65	49
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9	< 69	- 4
10	71	87
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6	128	126
7	< 59	4
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10	65	66
11	126	127
12	< 70	8
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16	< 80	- 59
17	185	-201
	9 k 4	
0	132	128
1	115	109
2	< 64	11
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4	72	- 79
5	< 66	- 40
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7	< 69	- 34
8	106	78
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10	< 74	- 16
11	< 76	- 45
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13	123	135
	-9 k 4	
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2	143	-170
3	57	54
4	135	147
5	155	-160
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7	91	- 81
8	231	235
9	81	- 67
10	94	- 98
11	103	83
12	162	170
	10 k 4	
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1	99	-101
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3	< 68	45
4	< 69	- 50
5	< 70	- 35
6	78	- 95
7	< 72	- 16
8	181	208
	-10 k 4	
0	92	89
1	193	220
2	49	34
3	89	-99
4	< 62	22
5	63	- 67
6	179	108
7	169	194
8	140	-147
9	< 69	- 28
10	< 71	- 13
11	< 73	26
12	< 75	- 36
13	145	170
14	< 80	29
15	90	93
	11 k 4	
0	54	66
1	115	90
2	121	-140
3	< 74	43
4	< 75	64
5	< 76	29
6	< 77	- 34
7	< 79	6
8	86	112
	-11 k 4	
0	64	- 61
1	105	105
2	217	235
3	< 66	- 52
4	< 67	5
5	< 68	56
6	85	- 80
7	139	-139
8	< 72	54
9	< 74	- 9
10	< 76	98
11	103	-107
12	113	-104
	12 k 4	
0	119	114
1	113	118
	-12 k 4	
0	90	75
1	< 68	- 55
2	< 69	44
3	< 70	- 27
4	105	-113
5	< 73	13
6	166	190
7	< 75	- 27
8	< 77	- 48
9	89	64
10	91	79
	-13 k 4	
0	130	159
1	56	- 65
2	< 73	- 65
3	< 73	- 56
4	< 74	- 37
5	< 75	44
6	121	-112
	-14 k 4	
0	< 76	- 63
1	70	71
2	61	58
3	< 77	- 71
4	< 78	- 61
5	< 79	36
6	107	-116
	-15 k 4	
0	109	99
	0 k 5	
1	153	154
2	86	-120
3	153	215
4	101	-105
5	181	-201
6	141	141
7	70	- 67
8	127	111
9	< 40	- 19
10	61	- 61
11	235	-226
12	92	- 84
13	< 47	- 16
14	75	57
15	< 52	- 49
16	86	63
17	< 56	25
18	< 58	49
19	149	155
20	89	- 79
	1 k 5	
1	78	89
2	280	-343
3	35	- 45
4	46	- 41
5	45	- 55
6	189	-186
7	< 34	- 7
8	< 36	- 29
9	98	101
10	< 43	15
11	44	51
12	111	-119
13	48	- 41
14	155	153
15	< 52	- 30
16	205	211
	-1 k 5	
1	87	67
2	< 27	21
3	103	-124
4	38	- 38
5	63	56
6	371	338
7	< 33	0
8	227	208
9	38	- 40
10	162	-157
11	131	104
12	114	-112
13	96	- 88
14	140	-134
15	< 51	1
16	< 54	- 38
17	< 56	31
18	< 58	- 16
19	< 60	- 28
20	117	-124
	2 k 5	
1	61	- 67
2	31	26
3	256	-276
4	95	- 91
5	< 32	- 17
6	164	163
7	64	65
8	84	91
9	140	142
10	98	- 99
11	232	240
12	< 46	- 15
13	73	- 73
	-2 k 5	
1	121	-149
2	268	-304
3	126	-136
4	79	85
5	44	42
6	< 30	11
7	132	100
8	124	102
9	145	129
10	< 40	40
11	188	153
12	204	-180
13	58	54
14	82	82
15	< 51	22
16	176	156
17	63	- 40
18	56	- 83
19	96	-108
	3 k 5	
1	109	120
2	72	74
3	97	119
4	51	48
5	184	-201
6	206	217
7	< 37	14
8	145	139
9	113	116
10	38	- 37
11	106	-105
12	72	- 70
13	50	- 39
14	58	- 65
	-3 k 5	
1	62	- 71
2	198	-226
3	143	149
4	237	-244
5	137	-109
6	52	- 37
7	< 34	3
8	< 36	- 10
9	< 39	16
10	106	- 87
11	207	-181
12	56	- 40
13	116	112
14	155	150
15	< 52	- 3
16	177	160
	4 k 5	
1	205	213
2	168	-175
3	< 34	19
4	< 35	40
5	93	-110
6	104	-118
7	63	- 79
8	41	- 36
9	< 43	29
10	< 45	43
11	79	- 81
12	90	-102
13	115	-125
14	51	62
15	62	- 55
16	99	84
17	98	95
18	68	- 50
	-4 k 5	
1	193	195
2	< 25	28
3	50	46
4	148	-131
5	166	136
6	283	225
7	86	- 77
8	116	105
9	315	-243
10	193	-159
11	< 44	- 44
12	46	- 30
13	118	- 92
14	< 51	- 53
15	< 52	24
16	< 55	19
17	< 57	25
18	< 59	45
19	< 61	14
20	110	-115
	5 k 5	
1	50	52
2	< 36	- 20
3	171	-187
4	147	-162
5	< 39	- 43
6	< 41	- 33
7	< 42	23
8	< 44	- 32
9	79	90
10	47	- 48
11	148	171
12	93	99
13	99	-111
14	< 54	52
15	< 56	- 16
16	59	80
	-5 k 5	
1	110	-108
2	121	-122
3	104	- 84
4	294	246
5	163	135
6	205	148
7	< 37	6
8	199	155
9	58	- 48
10	71	64
11	94	75
12	234	-196
13	73	51
	6 k 5	
1	39	- 29
2	86	95
3	< 40	6
4	< 41	9
5	150	-158
6	96	92
7	84	76
8	< 46	26
9	175	201
10	42	- 35
	-6 k 5	
1	258	-272
2	160	-145
3	99	75
4	132	-109
5	< 35	- 13
6	< 37	- 29
7	100	80
8	< 41	0
9	106	86
10	84	- 55
11	< 46	- 41
12	59	- 43
13	243	228
14	74	66
15	55	29
16	80	66
17	125	-117
	7 k 5	
1	93	92
2	< 42	- 9
3	< 43	11
4	166	167
5	85	- 87
6	< 45	- 9
7	< 46	- 37
8	< 48	5
9	< 49	36
10	77	75
11	53	- 58
12	52	- 76
	-7 k 5	
1	55	48
2	< 35	- 22
3	65	48
4	278	-241
5	193	188
6	56	38
7	54	- 45
8	< 42	- 24
9	246	-212
10	125	-105
11	< 48	- 25
12	117	96
13	< 51	- 3
14	54	65
15	< 55	42
16	< 57	75
17	< 59	- 12
18	107	115
	8 k 5	
1	151	144
2	< 45	19
3	69	- 53
4	74	- 71
5	< 47	12
6	80	- 63
7	< 54	- 34
8	< 51	- 43
9	< 52	- 28
10	< 53	- 6
11	< 55	38
12	86	93
13	120	-137
	-8 k 5	
1	< 38	20
2	61	- 71
3	< 39	19
4	175	184
5	157	153
6	< 42	36
7	94	- 82
8	45	45
9	213	-205
10	59	39
11	< 49	- 47
12	99	-107
13	< 53	- 13
14	< 55	- 28
15	< 57	47
16	< 59	0
17	< 61	- 3
18	99	- 97
	9 k 5	
1	< 48	- 38
2	49	50
3	< 48	- 11
4	78	- 78
5	100	-100
6	56	- 54
7	70	40
8	< 53	- 67
9	98	113
	-9 k 5	
1	159	-174
2	< 41	14
3	104	109
4	91	95
5	< 43	3
6	63	66
7	46	56
8	< 47	42
9	< 48	38
10	< 50	5
11	< 51	- 45
12	< 53	- 49
13	175	182
14	< 57	- 39
15	< 58	- 22
16	< 61	- 64
17	113	-107
	10 k 5	
1	< 51	- 15
2	< 51	36
3	< 51	- 24
4	134	141
5	< 55	- 52
6	< 53	- 18
7	< 54	15
8	< 55	- 6
9	85	74
10	96	78
	-10 k 5	
1	110	-122
2	< 44	39
3	< 45	- 43
4	148	-171
5	105	100
6	< 47	- 3
7	< 48	20
8	< 49	- 44
9	< 51	- 51
10	< 52	- 47
11	54	66
12	136	125
13	64	80
	11 k 5	
1	107	93
2	77	68
	-11 k 5	
1	< 46	29
2	53	- 58

Table 4. Continued.

3	< 47	26	8	68	54		-5 k 6		8	253	-229	1	< 51	37	3	< 24	- 29	2	< 35	27
4	< 48	30	9	57	- 50	0	210	239	9	118	-127	2	< 51	- 52	4	180	183	3	57	- 50
5	123	126	10	171	148	1	290	-304	10	< 48	- 15	3	< 51	- 49	5	150	-140	4	94	- 82
6	108	-119	11	82	62	2	37	29	11	< 50	21	4	< 52	- 5	6	< 32	3	5	161	-154
7	51	- 54	12	< 45	20	3	139	130	12	77	- 72	5	< 52	37	7	84	70	6	146	127
8	82	- 75	13	251	-236	4	49	- 39	13	98	- 99	6	101	122	8	46	33	7	100	90
9	138	-160	14	129	-116	5	< 31	21	14	61	- 45	7	< 58	36	9	238	233	8	79	75
	-12 k 5		15	118	106	6	46	33	15	187	198	8	95	- 91	10	122	116	9	159	171
1	< 49	- 35	16	103	82	7	310	276		9 k 6		9	< 60	- 24	11	< 45	37	10	93	- 83
2	70	68	17	190	-177	8	208	-180	0	124	-126	10	69	86	12	99	-103	11	68	63
3	125	133		3 k 6		9	120	- 91	1	121	129		0 k 7		13	< 49	7		8 k 7	
4	98	116	0	215	196	10	< 41	6	2	< 49	8	1	81	- 80	14	< 52	- 11	1	126	-101
5	< 51	8	1	156	141	11	< 43	10	3	< 50	32	2	< 22	- 20	15	< 54	- 42	2	82	74
6	< 52	22	2	108	110	12	87	- 78	4	< 50	15	3	< 25	- 7	16	79	- 74		-8 k 7	
7	< 53	- 12	3	54	- 61	13	229	-220	5	< 51	55	4	34	40		4 k 7		1	89	80
8	< 54	10	4	< 34	- 5	14	113	-105	6	< 51	- 20	5	129	-130	1	88	- 78	2	111	-112
9	< 55	- 41	5	93	97	15	138	134	7	97	- 83	6	172	-177	2	52	54	3	138	-142
10	< 57	45	6	215	-230	16	74	69	8	86	88	7	85	75	3	151	-159	4	135	-143
11	101	-109	7	155	-171	17	131	-130	9	77	74	8	123	-128	4	64	65	5	53	40
	-13 k 5		8	154	158		6 k 6			-9 k 6		9	197	202	5	100	94	6	< 42	- 30
1	75	-102	9	140	137	0	< 39	14	0	41	33	10	104	99	6	97	- 95	7	< 44	9
2	97	119	10	146	-162	1	193	191	1	98	- 86	11	39	38	7	< 43	21	8	< 46	1
	0 k 6		11	< 47	- 56	2	65	68	2	< 41	- 17	12	< 48	2	8	55	- 67	9	< 47	34
0	118	142	12	115	-100	3	64	62	3	< 41	25	13	< 50	44	9	< 45	43	10	68	- 61
1	< 18	9	13	99	95	4	< 41	4	4	213	209	14	69	78	10	74	80	11	96	110
2	< 33	3	14	59	- 64	5	143	147	5	207	185		1 k 7		11	136	127	12	< 53	20
3	189	-241	15	99	- 88	6	105	-100	6	212	-175	1	35	- 1	12	73	71	13	87	- 84
4	< 27	- 27	16	< 57	8	7	86	- 86	7	92	92	2	119	132		-4 k 7			9 k 7	
5	< 29	3	17	< 59	46	8	115	124	8	121	99	3	156	-174	1	54	- 44	1	59	- 41
6	275	-281	18	83	80	9	128	136	9	85	97	4	168	175	2	< 36	21	2	< 52	40
7	255	-238	19	< 65	- 27	10	79	- 70	10	178	-198	5	43	- 52	3	55	- 49	3	99	79
8	330	297	20	117	126	11	< 50	- 28	11	104	-101	6	< 34	21	4	196	-192	4	87	78
9	74	54		-3 k 6		12	< 51	- 43		10 k 6		7	< 37	- 4	5	192	-174		-9 k 7	
10	122	-111	0	< 21	- 25	13	< 53	41	0	< 53	52	8	< 39	6	6	50	- 49	1	99	105
11	134	-112	1	64	68	14	< 55	- 1	1	< 53	- 11	9	< 42	47	7	80	74	2	142	-141
12	< 46	- 15	2	125	-145	15	151	-154	2	< 53	- 43	10	69	70	8	< 39	- 31	3	52	48
13	153	151	3	223	-232		-6 k 6		3	132	128	11	121	124	9	165	159	4	< 43	35
14	85	- 69	4	< 26	7	0	46	- 45	4	85	82	12	< 48	22	10	72	- 68	5	66	- 61
15	59	53	5	101	87	1	93	- 95	5	< 54	14	13	67	- 67	11	68	55	6	< 45	- 8
16	< 55	24	6	265	-234	2	121	-119	6	< 55	- 33	14	94	- 98	12	107	113	7	47	- 47
17	134	121	7	139	-111	3	94	- 82	7	< 56	- 44	15	< 55	- 82	13	< 50	- 14	8	< 48	26
18	< 59	38	8	538	409	4	153	133	8	< 57	- 15	16	102	-104	14	56	45	9	< 49	19
19	< 61	- 25	9	95	67	5	289	237	9	< 58	29		-1 k 7			5 k 7		10	< 51	28
20	106	-110	10	< 37	- 5	6	249	-204	10	98	- 76	1	156	138	1	54	- 30	11	114	-111
21	< 65	44	11	177	-160	7	115	86		-10 k 6		2	78	89	2	205	184	12	117	-118
22	77	-115	12	159	125	8	342	300	0	207	-265	3	50	51	3	< 41	26	13	80	- 59
	1 k 6		13	77	67	9	141	122	1	140	143	4	175	-162	4	42	45	14	67	69
0	137	168	14	< 50	- 34	10	85	- 67	2	44	- 25	5	151	-137	5	37	29		10 k 7	
1	263	-232	15	75	64	11	176	-171	3	131	-149	6	101	- 89	6	67	61	5	88	82
2	225	-210	16	< 55	14	12	167	151	4	< 45	- 29	7	< 35	- 21	7	< 45	28		-10 k 7	
3	133	165	17	85	77	13	76	- 63	5	107	101	8	80	- 72	8	< 47	7	1	< 44	16
4	119	-126	18	65	- 65	14	< 51	- 17	6	86	80	9	< 40	19	9	< 48	- 26	2	< 45	27
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7	< 36	49	21	< 65	17	17	< 56	- 27	9	< 51	18	12	178	179	12	< 54	78	5	82	- 75
8	181	171	22	150	-190	18	102	-100	10	75	80	13	88	- 84	13	< 55	14	6	149	169
9	63	- 58		4 k 6			7 k 6		11	98	-123	14	< 52	28	14	97	-116	7	< 49	26
10	181	175	0	273	259	0	213	204	12	< 55	55	15	< 54	- 29	15	< 59	8	8	99	103
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12	104	87	2	103	- 91	2	< 41	- 19	14	103	103	17	< 58	45		-5 k 7		10	71	- 75
13	117	-115	3	110	106	3	134	126	15	101	-116	18	67	94	1	202	243	11	< 55	- 49
14	120	-107	4	< 33	- 33	4	74	71	16	70	- 68		2 k 7		2	66	- 50	12	55	- 64
15	169	172	5	217	-204	5	100	-102	17	101	90	1	115	133	3	91	- 91		-11 k 7	
16	124	85	6	48	- 49	6	47	- 58		11 k 6		2	163	189	4	41	- 75	1	< 47	- 38
17	108	-110	7	141	-142	7	123	-117	0	< 55	- 3	3	114	107	5	< 33	27	2	48	- 50
	-1 k 6		8	99	86	8	< 49	- 11	1	< 55	26	4	< 32	- 12	6	79	- 58	3	115	-131
0	196	213	9	66	- 56	9	< 50	- 15	2	< 55	38	5	42	- 36	7	85	- 74	4	< 49	- 48
1	167	-159	10	< 45	37	10	95	- 94	3	< 56	28	6	< 36	20	8	49	- 37	5	50	52
2	288	318	11	145	145	11	88	89	4	< 56	9	7	< 38	- 34	9	43	- 45	6	80	79
3	108	-134	12	< 48	35	12	< 55	- 13	5	95	- 87	8	< 41	- 21	10	44	- 43	7	< 52	51
4	223	-252	13	< 50	- 40	13	< 57	- 58	6	71	66	9	71	- 68	11	< 46	23	8	68	64
5	75	69	14	115	-112	14	76	- 91		-11 k 6		10	< 45	- 24	12	< 49	12	9	< 54	28
6	114	100	15	146	162	15	66	60	0	58	- 64	11	99	88	13	191	-188	10	51	- 51
7	194	167	16	96	92		-7 k 6		1	133	-148	12	125	129	14	< 53	21	11	102	130
8	200	-164	17	< 58	- 51	0	226	-252	2	< 47	- 28	13	68	- 68	15	< 55	- 47		-12 k 7	
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10	108	96	19	115	95	2	< 35	18	4	< 48	24	15	< 55	- 23	17	106	130	2	158	-162
11	85	- 71		-4 k 6		3	387	-340	5	119	-136	16	103	- 98		6 k 7		3	51	7
12	260	-249	0	54	55	4	125	-112	6	125	147		-2 k 7		1	< 42	9	4	< 52	- 34
13	71	65	1	86	95	5	< 38	0	7	< 55	28	1	218	223	2	< 43	26	5	< 53	4
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15	139	-127	3	384	-348	7	78	66	9	85	- 81	3	100	-117	4	59	56		-13 k 7	
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	2 k 6		7	87	63	11	140	-125	2	< 50	2	7	89	- 83	8	< 49	- 47	4	< 54	- 45
0	42	32	8	188	-144	12	< 50	- 4	3	< 50	3	8	< 37	11	9	83	- 77	5	< 55	- 17
1	163	173	9	76	- 71	13	181	169	4	155	181	9	< 40	- 37	10	73	60	6	79	77
2	117	129	10	89	88	14	112	95	5	< 51	7	10	< 42	23	11	131	-131		-14 k 7	
3	69	75	11	106	- 98	15	< 56	- 15	6	100	- 111	11	< 44	34		-6 k 7		6	99	106
4	271	-278	12	192	-173	16	65	- 78	7	< 53	- 27	12	< 47	- 14	1	106	112		-15 k 7	
5	58	55	13	206	188	17	160	195	8	< 54	2	13	197	-189	2	50	- 44	1	83	- 62
6	152	152	14	< 49	20		8 k 6		9	< 55	40	14	92	- 97	3	41	39	2	83	- 79
7	166	156	15	< 51	1	0	69	- 67	10	167	-192	15	59	- 50	4	186	186		0 k 8	
8	77	- 69	16	< 55	- 68	1	74	66		-13 k 6		16	54	- 63	5	130	-125	6	97	87
9	36	- 41	17	204	204	2	< 47	- 3	0	88	-112	17	110	131	6	97	87	7	40	- 20
10	208	-199	18	141	148	3	< 47	25	1	100	144		3 k 7		7	< 40	- 20	1	120	131
11	< 45	- 1		5 k 6		4	94	- 92	2	< 53	34	1	< 32	- 16	8	102	93	2	129	-122
12	156	-147	0	95	- 84	5	111	-146	3	< 53	- 37	2	< 33	- 14	9	79	78	3	67	75
13	< 49	- 19	1	145	134	6	115	98	4	< 54	54	3	99	93	10	64	71	4	70	75
14	< 52	5	2	< 37	- 23	7	< 50	- 38	5	87	98	4	< 35	- 7	11	76	- 74	5	158	185
15	220	-195	3	91	88	8	82	- 82	6	< 55	32	5	81	- 87	12	153	-153	6	< 37	- 21
16	75	- 56	4	228	-231	9	65	- 66	7	< 56	48	6	198	-214		7 k 7		7	186	-205
17	< 53	- 31	5	80	- 76	10	91	100	8	< 57	- 53	7	< 40	- 8	1	< 45	- 6	8	117	113
18	109	117	6	130	138	11	106	107	9	< 58	31	8	150	-153	2	< 46	- 30	9	186	214
	-2 k 6		7	< 41	30		-8 k 6		10	< 59	- 38	9	< 44	12	3	< 46	- 38	10	< 48	- 2
0	200	211	8	< 43	- 22	0	101	106	11	< 60	- 78	10	66	80	4	< 47	- 23	11	69	- 41
1	267	276	9	57	- 67	1	268	-263	12	< 62	7	11	77	- 77	5	117	103	12	98	94
2	111	-154	10	226	224	2	69	62	13	< 63	30	12	< 50	47	6	132	-111	13	< 55	23
3	194	220	11	100	82	3	< 39	- 34	14	< 64	58	13	< 52	28	7	< 50	- 16	14	< 57	7
4	135	-141	12	< 50	- 31	4	< 40	32	15	114	-129	14	73	83	8	76	- 76	15	105	-113
5	74	60	13	< 51	23	5	147	-125		-14 k 6			-3 k 7			-7 k 7		16	< 63	22
6	< 28	8	14	< 53	45	6	105	109	0	88	-101	1	< 18	- 31	1	82	- 77	17	< 64	- 35
7	383	387	15	104	- 97	7	112	108				2	< 21	4				18	79	- 96

Table 4. Continued.

	1 k 8		3 k 8		2 166 163	10 < 62 0	15 < 67 65		-14 k 8		7 262 214				
0 175 201	0 172 -145	3 58 58	11 < 64 29	16 132 100	7 161 145	3 104 - 89									
1 < 29 13	1 82 66	4 < 48 37	12 136 126		8 < 68 - 69	2 235 -161									
2 86 - 85	2 88 - 81	5 43 - 45		10 k 8	9 96 - 78	1 221 147									
3 178 211	3 65 - 65	6 70 60	-7 k 8	0 < 63 47											
4 117 138	4 89 89	7 89 94	0 < 39 - 75	1 < 63 - 52	-15 k 8	1 85 - 98									
5 79 - 84	5 64 56	8 136 -131	1 133 139	2 < 63 - 66	0 59 - 55	2 67 61									
6 < 39 1	6 < 45 7	9 < 55 - 47	2 209 207	3 < 63 - 53	1 104 - 56										
7 81 84	7 213 -249	10 85 - 58	3 56 46	4 91 66	h 0 10	h 3 9									
8 107 -103	8 < 49 46	11 55 42	4 180 -187		15 143 151	9 91 -108									
9 87 - 83	9 124 151	12 104 - 86	5 136 136	-10 k 8	14 < 55 - 26	7 123 136									
10 106 -119	10 < 53 3	13 < 63 - 17	6 < 45 2	0 < 50 14	13 < 55 - 81	5 83 - 89									
11 127 128	11 < 55 - 52	14 99 92	7 < 41 23	1 78 68	12 119 162	3 172 124									
12 117 -113	12 95 96	15 < 67 - 39	8 < 49 54	2 229 215	11 < 52 33	1 77 33									
13 89 -105	-3 k 8	16 79 - 82	9 76 60	3 93 - 69	10 150 -171	7 66 63									
14 71 - 46	0 219 191	-5 k 8	10 90 90	4 105 -101	9 66 70	0 < 56 18									
15 110 103	1 133 -128	0 140 169	11 56 - 57	5 95 95	8 < 49 29	1 < 57 11									
16 105 -107	2 55 - 45	1 72 - 71	12 147 -143	6 < 54 - 35	7 159 -172	2 62 58									
17 79 - 49	3 97 111	2 70 - 83	13 < 60 14	7 < 55 - 13	6 < 48 4	3 < 58 - 22									
	4 77 64	3 74 91	14 58 78	8 < 57 2	5 < 48 - 81	4 < 59 11									
-1 k 8	5 200 216	4 72 - 71	15 161 -157	9 < 58 52	4 154 -161	5 66 86									
0 439 -324	6 135 -121	5 251 -285	16 149 -120	10 < 60 - 8	3 < 48 48	h 3 10									
1 63 121	7 167 -186	6 56 35	17 < 69 - 26	11 67 - 79	2 137 -122	11 99 83									
2 143 119	8 71 74	7 < 43 27	18 127 120	12 155 -157	1 284 -229	10 < 65 18									
3 < 27 6	9 193 216	8 < 45 28		13 < 65 59	0 93 96	9 < 64 - 44									
4 138 -164	10 121 -103	9 173 -192	8 k 8	14 < 67 31	1 < 47 22	8 173 169									
5 147 -163	11 < 51 - 36	10 79 75	0 150 -123	15 < 69 - 56	2 303 -231	7 < 62 14									
6 91 89	12 < 54 11	11 193 208	1 < 56 2	16 < 70 - 76	3 < 49 46	6 < 62 78									
7 120 -128	13 < 56 - 4	12 < 55 26	2 67 56	17 < 71 40	4 153 141	5 196 165									
8 < 42 - 1	14 98 - 92	13 < 58 4	3 < 57 40	18 116 129	5 135 -111	4 < 61 - 47									
9 56 - 53	15 110 -125	14 102 - 93	4 < 58 17			3 215 -173									
10 112 117	16 64 74	15 122 103	5 < 58 9	11 k 8	h 0 12	2 < 60 - 40									
11 87 90			6 < 59 49	0 97 - 84	10 70 - 84	1 93 69									
12 77 - 71	4 k 8	6 k 8	7 150 128	1 < 66 - 23	9 < 56 96	0 137 -145									
13 126 108	0 < 42 10	0 104 - 85		2 < 66 1	8 68 - 58	1 80 - 72									
14 171 178	1 < 42 4	1 < 49 8	-8 k 8	3 < 66 - 14	7 < 55 148	2 < 62 10									
15 < 60 - 28	2 200 -178	2 < 50 21	0 < 43 52	4 < 67 - 15	6 105 94	3 < 63 - 76									
16 137 -135	3 162 149	3 122 -114	1 70 - 61	5 < 67 - 20	5 55 77	4 < 64 - 55									
	4 114 124	4 87 77	2 117 -111	6 < 68 21	4 95 -108	5 70 - 36									
2 k 8	5 < 46 - 5	5 < 52 24	3 103 97	7 123 80	3 < 55 30										
0 205 -197	6 < 48 27	6 < 53 - 6	4 143 -149		2 106 125	h 3 12									
1 79 65	7 106 93	7 187 -175	5 127 -131	-11 k 8		0 90 -122									
2 230 196	8 < 51 - 36	8 < 56 - 45	6 66 49	0 < 53 50	h 1 9	1 < 69 56									
3 < 35 7	9 < 53 - 30	9 86 80	7 164 155	1 < 53 - 41	1 232 -181	2 < 70 73									
4 < 37 - 34	10 < 55 - 39	10 68 - 58	8 72 72	2 < 53 - 22	2 148 -136	3 < 70 - 90									
5 147 -162	11 76 70		9 132 -137	3 99 91	3 109 - 97	4 < 70 15									
6 80 67	12 121 126	-6 k 8	10 181 167	4 126 -103		5 93 102									
7 39 - 39	13 97 - 90	0 315 330	11 137 133	5 < 56 - 9	h 1 10										
8 114 -137	14 73 - 50	1 < 34 23	12 55 42	6 < 57 35	2 110 - 96	h 4 9									
9 67 - 67	15 < 66 - 33	2 45 - 29		7 209 211	5 127 -103	0 156 157									
10 < 50 - 23	16 < 68 78	3 < 37 - 14	9 k 8	8 < 59 - 7		1 68 - 90									
11 92 92	17 80 - 79	4 39 44	0 55 - 45	9 119 - 99	h 2 9	2 84 - 85									
12 114 -108	18 92 -106	5 95 86	1 < 49 - 9	10 100 94	11 88 99	3 101 101									
13 78 72		6 162 -168	2 < 60 50	11 < 64 41	10 < 54 8	4 < 60 - 10									
14 129 138	-4 k 8	7 214 -219	3 < 60 - 61	12 < 65 - 13	9 < 54 - 5	5 74 - 83									
15 < 62 0	0 287 -290	8 74 67	4 < 61 44	13 94 - 86	8 159 170										
16 100 -107	1 122 161	9 121 117	5 79 71		7 63 84										
	2 94 110	10 149 -132	6 < 62 - 6	-12 k 8	6 < 51 26										
-2 k 8	3 57 58	11 < 54 - 34	7 72 - 44	0 94 96	5 127 125										
0 367 300	4 192 -225	12 < 56 - 32	8 65 - 54	1 89 - 88	4 131 120										
1 < 15 - 26	5 < 35 11	13 59 37		2 131 -132	3 < 49 2										
2 < 33 - 22	6 73 68	14 141 -150	-9 k 8	3 70 - 58	2 < 49 - 47										
3 130 170	7 42 - 47	15 < 63 - 1	0 209 227		1 < 50 - 51										
4 65 66	8 92 93	16 118 112	1 80 - 76	-13 k 8	0 < 50 9										
5 216 -254	9 < 46 16		2 120 -103	0 < 58 - 39	1 < 50 11										
6 < 36 - 6	10 170 161	7 k 8	3 100 -100	1 < 59 - 7	2 < 51 - 47										
7 < 39 - 1	11 < 52 17	0 < 53 - 13	4 < 48 22	2 109 105	3 < 52 - 44										
8 90 - 84	12 75 - 69	1 65 - 44	5 < 49 - 16	3 147 -143	4 < 53 19										
9 166 -168	13 < 57 44	2 127 -156	6 116 -118	4 < 61 - 52	5 < 54 - 55										
10 81 - 88	14 145 156	3 < 54 11	7 183 -181	5 < 62 25	6 117 - 97										
11 180 201	15 143 -138	4 107 88	8 129 121	6 < 63 - 39											
12 < 53 - 12	16 144 -150	5 < 55 - 26	9 < 56 45	7 < 64 - 44	h 2 10										
13 < 56 - 37		6 < 56 18	10 < 58 - 35	8 < 65 19	9 129 -163										
14 115 -126	5 k 8	7 < 58 37	11 < 59 - 32	9 < 66 33	8 < 56 48										
15 < 61 48	0 137 -128	8 < 59 - 5	12 < 61 32	10 < 67 - 1	7 135 154										
16 99 102	1 < 46 34	9 < 60 - 22	13 < 63 43	11 < 68 - 73	6 127 109										
			14 133 -128	12 75 - 72	5 85 - 76										
				13 81 78											

using anisotropic temperature factors for the mercury atoms resulted in a final R factor of 0.117 for the 2350 observed reflections. In the final cycle all shifts in parameters were less than one tenth of the calculated standard deviations.

The final parameter values are given in Table 3, and a comparison between observed and calculated structure factors is given in Table 4. Because of the presence of absorption errors in the observed F values the anisotropic temperature factors have no physical meaning and for this reason, only the isotropic temperature factors are given in Table 3.

The final parameter values were used for the calculation of a three-dimensional electron density map and a corresponding difference map. In the electron density map the peak heights were between 320 and 366 e/Å^3 for the mercury atoms and 50 and 54 e/Å^3 for the chlorine atoms. The average peak

height for the oxygens was 15 e/Å^3 with a lowest value (for O_6) of 10 e/Å^3. In the difference map all peaks, except in the immediate vicinity of the mercury positions, were below 4 e/Å^3.

DISCUSSION OF THE STRUCTURE

Interatomic distances and bond angles are given in Table 5. Projections of the structure along the *a* and *c* axes are shown in Fig. 1.

Each mercury in the structure forms two short bonds to surrounding oxygens with bond lengths of 1.93 to 2.10 Å, (average value 2.02 Å). The bonds to the non-bridging oxygens (average bond length 1.95 Å) are shorter,

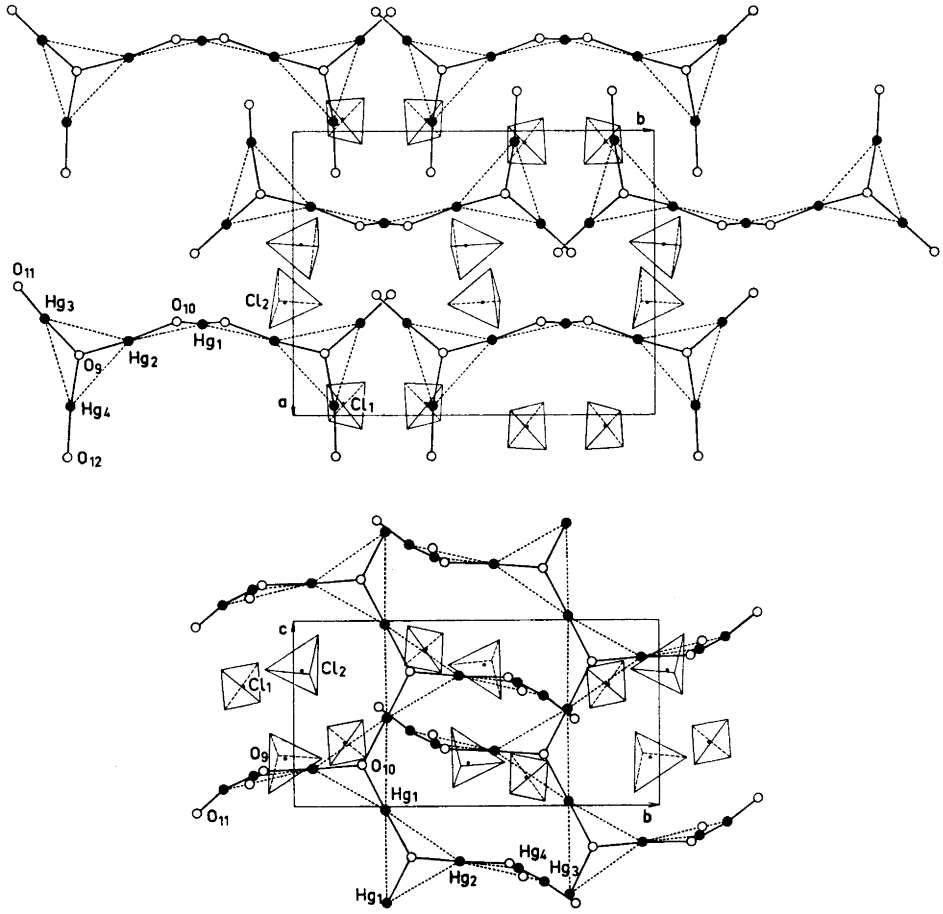

Fig. 1. Projections of the structure along the *c* and *a* axes. Full-drawn lines indicate covalent Hg – O bonds. Mercury atoms, which share covalently bonded oxygens, are connected by dotted lines.

and probably significantly so, than the bonds to the bridging oxygens (average bond length 2.04 Å). The corresponding O – Hg – O angles are close to 180° (Table 5). Other Hg – O distances are larger than about 2.7 Å and probably

Table 5. Interatomic distances and angles.

Hg – O distances (< 3.5 Å)

$Hg_1 - O_{10}$	1.99 (3) Å	$Hg_2 - O_9$	1.98 (3) Å
$- O_{10}$	2.10 (3)	$- O_{10}$	2.06 (3)
$- O_{12}$	2.71 (4)	$- O_{12}$	2.65 (4)
$- O_8$	2.78 (9)	$- O_8$	2.66 (8)
$- O_{11}$	2.79 (4)	$- O_6$	2.70 (7)
$- O_5$	2.83 (4)	$- O_1$	2.84 (6)
$- O_4$	3.14 (5)	$- O_5$	2.85 (4)
$Hg_3 - O_{11}$	1.96 (4) Å	$Hg_4 - O_{12}$	1.93 (4) Å
$- O_9$	2.05 (3)	$- O_9$	2.06 (3)
$- O_{11}$	2.81 (4)	$- O_1$	2.72 (6)
$- O_6$	2.88 (7)	$- O_2$	2.91 (5)
$- O_2$	3.10 (5)	$- O_3$	2.92 (5)
$- O_7$	3.17 (6)	$- O_1$	2.99 (6)
$- O_2$	3.17 (5)	$- O_4$	3.13 (5)
$- O_8$	3.49 (8)	$- O_4$	3.14 (6)

O – Hg – O angles

$O_{10} - Hg_1 - O_{10}$ 171.8° (18)	$O_9 - Hg_2 - O_{10}$ 172.8° (12)
$O_9 - Hg_3 - O_{11}$ 172.9° (14)	$O_9 - Hg_4 - O_{12}$ 171.9° (15)

Hg – Hg distances (< 4.5 Å)

$Hg_1 - Hg_2$	3.386 (2) Å	$Hg_2 - Hg_1$	3.386 (2) Å
$- Hg_2$	3.507 (2)	$- Hg_4$	3.398 (3)
$- 2Hg_1$	3.612 (3)	$- Hg_1$	3.507 (2)
		$- Hg_3$	3.514 (3)
$- Hg_3$	4.141 (3)		
$- Hg_4$	4.345 (3)	$- Hg_4$	3.943 (5)
$Hg_3 - Hg_2$	3.514 (3) Å	$Hg_4 - Hg_2$	3.398 (3) Å
$- Hg_4$	3.515 (3)	$- Hg_3$	3.515 (3)
$- 2Hg_3$	4.070 (3)	$- Hg_4$	3.942 (4)
$- Hg_1$	4.141 (3)	$- Hg_2$	3.943 (5)
		$- Hg_1$	4.345 (3)

Hg – O distances involving $O_9 - O_{12}$ (< 4.5 Å):

$O_9 - Hg_2$	1.98 (3) Å	$O_{10} - Hg_1$	1.99 (3) Å
$- Hg_4$	2.05 (3)	$- Hg_2$	2.06 (3)
$- Hg_3$	2.05 (3)	$- Hg_1$	2.10 (3)
$- Hg_3$	4.38 (3)	$- Hg_3$	4.21 (3)
$- Hg_4$	4.45 (3)		
$O_{11} - Hg_3$	1.96 (4) Å	$O_{12} - Hg_4$	1.93 (4) Å
$- Hg_1$	2.79 (4)	$- Hg_2$	2.65 (4)
$- Hg_3$	2.81 (4)	$- Hg_1$	2.71 (4)
$- Hg_1$	4.48 (4)	$- Hg_4$	4.14 (4)
		$- Hg_1$	4.26 (4)

Table 5. Continued.

Hg – O – Hg angles

$Hg_3 - O_9 - Hg_3$	121.0° (16)	$Hg_1 - O_{10} - Hg_1$	123.9° (16)
$Hg_2 - O_9 - Hg_4$	114.7 (15)	$Hg_1 - O_{10} - Hg_2$	113.2° (15)
$Hg_3 - O_9 - Hg_4$	117.8° (15)	$Hg_1 - O_{10} - Hg_2$	114.7 (15)

Cl – O distances in the perchlorate groups

$Cl_1 - O_1$	1.36 (6) Å	$Cl_2 - O_5$	1.42 (4) Å
$- O_2$	1.29 (5)	$- O_6$	1.41 (7)
$- O_3$	1.27 (6)	$- O_7$	1.43 (7)
$- O_4$	1.41 (6)	$- O_8$	1.60 (8)

correspond to non-bonding contacts. The formation of two linear covalent bonds from the mercury atom has been found in many other structures.[8] The corresponding Hg – O bond lengths are usually found to be close to 2.0 Å.[9]

Two types of covalently bonded oxygen atoms are present in the structure. The oxygens O_9 and O_{10} are each bound to three Hg atoms at distances between 1.98 and 2.10 Å, and O_{11} and O_{12} are each bound to only one Hg atom at distances of 1.96 Å and 1.93 Å. Besides being covalently bound to one Hg atom each of O_{11} and O_{12} is also in non-bonding contact with two other Hg atoms at distances varying between 2.65 and 2.81 Å (Table 5).

In addition to the 8 negative charges from the perchlorate groups, 24 more are needed to neutralize the positive charges of the 16 Hg atoms in the unit cell. These must be provided by the 16 covalently bound oxygen atoms ($O_9 - O_{12}$). It seems reasonable to assume that O_9 and O_{10}, which are each bound to three Hg atoms, represent O^{2-}, and O_{11} and O_{12}, which are each bound to only one Hg atom, represent OH^-. The correct formula for the compound should then be written $Hg_2OOHClO_4$.

The shortest Hg – Hg distances range from 3.39 to 3.61 Å (average value 3.50 Å) and occur between those mercury atoms, that are joined by the covalently bound oxygens O_9 and O_{10}. The next shortest Hg – Hg distances are longer than about 4.0 Å (Table 5.)

If only the mercury atoms and the covalently bound oxygen atoms are considered, the structure can be described as being built up from infinite one-dimensional complexes as illustrated in Figs. 1 and 2. Characteristic features in these complexes are the OHg_3 groups consisting of three Hg atoms at the corners of a triangle with an oxygen (O_9 or O_{10}) slightly above the center of

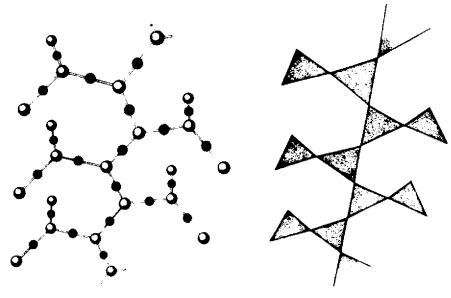

Fig. 2. A perspective view of one of the infinite one-dimensional complexes which can be distinguished in the structure when only the mercury atoms and the covalently bound oxygens are considered. Small filled circles indicate mercury atoms. Large circles indicate the oxygens O_9 and O_{10}, which are each bonded to three Hg atoms, or O_{11} and O_{12}, which are each bonded to only one Hg atom. To the right, the Hg_3-triangles of the OHg_3-groups are separately drawn.

the triangle. The complexes can be described as built up from such triangles sharing corners as shown in Fig. 2. Similar OHg_3 groups can be distinguished in several other basic salts of mercury. In Hg_3OCl_4 discrete $OHg_3Cl_3^+$ ions occur[10] with Hg–Hg distances of 3.53 Å and Hg–O distances of 2.05 Å, which are close to the values found here. The oxygen atom in the $OHg_3Cl_3^+$ ion is about 0.3 Å above the plane formed by the three Hg atoms.[11] This is found also in the present structure, where the O_9 and O_{10} atoms are about 0.3 Å (0.25 Å and 0.31 Å, respectively) above the plane of the three Hg atoms to which they are bound.

The average values for the Cl–O and O–O distances in the perchlorate groups are of the magnitude expected. The variations of the individual distances from the calculated mean are consistent with the estimated standard deviations.

As will be shown in a following paper the structure of $Hg_2OOHClO_4$ is closely related to that of the less basic $Hg_7O_4(OH)_2(ClO_4)_4$. The less basic salt is found also to be built up from infinite one-dimensional complexes, which can, in fact, be described as being formed by the condensation of two of the infinite complexes in $Hg_2OOHClO_4$.

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REFERENCES

1. Johansson, G. *Acta Chem. Scand.* **25** (1971) 2787, 2799.
2. Johansson, G. *Acta Chem. Scand.* **25** (1971) 1905.
3. Hayek, E. and Schnell, E. *Monatsh.* **85** (1954) 472.
4. Fischer, K. *Angew. Chem.* **48** (1935) 394.
5. Cromer, D. T. and Waber, J. T. *Acta Cryst.* **18** (1965) 104.
6. Cromer, D. T. *Acta Cryst.* **18** (1965) 17.
7. Hughes, E. W. *J. Am. Chem. Soc.* **63** (1941) 1737.
8. Grdenic, D. *Quart. Revs. Chem. Soc.* **19** (1965) 303.
9. Aurivillius, K. *Arkiv Kemi* **24** (1965) 151.
10. Weiss, A., Nagorsen, G. and Weiss, A. *Z. anorg. allgem. Chem.* **274** (1953) 151.
11. Aurivillius, K. *Arkiv Kemi* **22** (1964) 517, 537.

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