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Refinement of the Crystal Structure of Potassium Barium Hexathionate

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The crystal structure of potassium barium hexathionate, $K_2Ba(S_6O_6)_2$, has been refined by full-matrix least squares for 2375 independent non-zero reflections. The data were collected by means of a single-crystal diffractometer using Mo$K\alpha$ radiation (Nb-filtered). The refinement converged at a conventional R value of 0.020.

The space group is $P2/c$ (No. 13) with two formula units in a unit cell of dimensions $a = 11.591(4)$ Å, $b = 10.835(5)$ Å, $c = 9.145(3)$ Å, $\beta = 111.93(4)°$.

The six-membered sulphur chain of the hexathionate anion has the *cis-cis* rotational isomeric form. The bond lengths and angles, from one end of the chain to the other, are 2.119(1), 2.042(2), 2.056(2), 2.039(2), 2.110(1) Å, and 101.25(5)°, 110.20(5)°, 108.99(5)°, 99.95(5)°. The SSS/SSS dihedral angles are 109.4°, 89.0°, and 106.3°.

The crystal struetures of two salts of hexathionic acid have been published, both in 1965. In one of these salts, $K_2Ba(S_6O_6)_2$,[1] the anion occurs in the *cis-cis* rotational isomeric form, whereas in the other one, $[Co(en)_2Cl_2]_2S_6O_6 .H_2O$,[2] the anion has the *trans-trans* form. In the latter structure there was a tendency of variation in the lengths of the three middle S – S bonds, although the differences might not have been significant. Mainly to decide this point new sets of data have been recorded on a single-crystal diffractometer and refined by a full-matrix least squares program. The refinements and results are described in the present and a following paper.[3]

EXPERIMENTAL

The measurements were carried out on a Siemens automatic single-crystal diffractometer using Mo$K\alpha$ radiation (Nb-filtered) and a scintillation counter.

The crystals of $K_2Ba(S_6O_6)_2$ were prepared by Foss and Palmork.[4] The sample used had been kept for thirteen years in a refrigerator, and showed no signs of decomposition. The crystal used for measurements of unit cell dimensions and intensities was a prism along the c axis, bounded by (100), (110), and (1$\bar{1}$0), and terminated by ($\bar{1}$11). It was mounted with the c axis approximately parallel to the ϕ axis of the diffractometer, and oriented by measurements of θ,χ, and ϕ angles of six non-coplanar reciprocal vectors.

The five-value procedure and $\theta - 2\theta$ scan technique, with scan width of 0.70°, were used. The maximum scan time per degree was 24 sec.

Two reflections, 12 0 0 and 0 10 0, were measured two times each at intervals of 50 reflections. The intensities of these reflections decreased by 6 % during the data collection, and were used to bring the net intensities to a common scale.

Reflections were measured up to $\theta = 28°$, and only 215 of the 2590 independent reflections within this region were found to have net intensities below three times its standard deviation. These reflections were assigned an intensity equal to this limit, and labelled as unobserved.

Beside Lorentz and polarization corrections, the intensities were also corrected for absorption. The linear absorption coefficient for Mo$K\alpha$ is 34.7 cm^{-1}. The crystal used had a length along c of 0.330 mm, and the distances between the (100), between the (110), and between the (1$\bar{1}$0) boundary faces were 0.087, 0.130, and 0.130 mm, respectively. The number of Gaussian grid points used along the a, b, and c axes were 6, 6, and 12, respectively. The absorption factors, by which the intensities were multiplied, varied from 1.29 to 1.51.

The scattering factor curves used where those listed in *International Tables for X-Ray Crystallography*,[5] except for barium ion, for which the curve given by Thomas and Umeda[6] was used. The curves for barium, potassium, and sulphur were corrected for anomalous dispersion using the values given by Cromer,[7] and taking the amplitude as the corrected value.

The refinement was carried out with a full-matrix least squares program minimizing the function

$$r = \sum W(|F_o| - K|F_c|)^2$$

The intensity data were eventually corrected for secondary extinction with a program written by K. Åse of this Institute.

For further details concerning the data collection and the programs used, see Ref. 8.

The unit cell dimensions, calculated by means of a least squares program using the θ angles ($\theta = 21 - 28°$) of 15 reflections measured on the diffractometer, are $a = 11.591(4)$ Å, $b = 10.835(5)$ Å, $c = 9.145(3)$ Å, $\beta = 111.93(4)°$.

The space group is $P2/c$ (No. 13) with two $K_2Ba(S_6O_6)_2$ units per unit cell.[4]

REFINEMENT

The least squares refinement was started using the positional parameters given by Foss and Johnsen,[1] and individual isotropic thermal parameters that were the averaged values of those given for the two projections. Refinement on scale factor, positional parameters, and isotropic thermal parameters resulted in an R value ($\sum||F_o| - |F_c||/\sum|F_o|$) of 0.095. On using anisotropic thermal parameters for barium, potassium, and sulphur the R value was reduced to 0.031, and with anisotropic, thermal parameters also for the oxygen atoms, the refinement converged at $R = 0.022$.

For the reflections with highest intensities, the observed structure factors were considerable lower than the calculated ones. Secondary extinction corrections were therefore carried out. The expression given by Zachariasen [9] was used. With the absorption term equal to one, C was found to be 6.0×10^{-7}. The observed values of the structure factors now corresponded well to the calculated ones also for the strongest reflections.

The final R value was 0.020, with unobserved reflections included when $|F_c|$ is greater than the observable limit. There were no shifts of the parameters in the last refinement cycle.

A final difference electron density map showed no peaks higher than 0.4 e/Å^3.

Table 1. Atomic coordinates for potassium barium hexathionate. Origin at a centre of symmetry. Standard deviations are given in parentheses.

	x	y	z
Ba	0	0.01396(2)	¼
K(1)	½	0	½
K(2)	0	0.44987(8)	¼
S(1)	0.13933(6)	0.27403(5)	0.04470(7)
S(2)	0.33447(7)	0.28355(8)	0.16708(10)
S(3)	0.34815(9)	0.42062(8)	0.32588(9)
S(4)	0.40178(8)	0.34854(8)	0.54946(9)
S(5)	0.24695(8)	0.30389(7)	0.59363(10)
S(6)	0.25238(5)	0.10984(6)	0.57818(7)
O(1)	0.10136(21)	0.39894(17)	−0.00500(25)
O(2)	0.13175(21)	0.18877(19)	−0.07952(24)
O(3)	0.08578(18)	0.22999(17)	0.15501(23)
O(4)	0.36031(19)	0.06818(23)	0.70720(24)
O(5)	0.13276(16)	0.07734(17)	0.58622(20)
O(6)	0.25668(16)	0.07982(17)	0.42586(21)

Table 2. Thermal parameters expressed in the form exp $[-2\pi^2(h^2a^{-2}U_{11}+\cdots+2hka^{-1}b^{-1}U_{12}+\cdots)]$. All values have been multiplied by 10^4. Standard deviations are given in parentheses.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Ba	196(1)	202(1)	182(1)	0	0	77(1)
K(1)	284(5)	1270(12)	402(6)	169(6)	−366(7)	5(5)
K(2)	575(6)	254(4)	331(5)	0	0	156(4)
S(1)	300(3)	200(3)	274(3)	−33(3)	7(2)	88(3)
S(2)	302(4)	574(5)	549(5)	−72(4)	−40(4)	153(4)
S(3)	647(6)	387(4)	423(5)	−270(4)	39(4)	41(4)
S(4)	521(5)	554(5)	416(5)	−327(4)	56(4)	−15(4)
S(5)	653(6)	303(4)	574(5)	−119(4)	−124(4)	285(5)
S(6)	197(3)	279(3)	223(3)	−30(2)	32(2)	57(2)
O(1)	621(16)	250(10)	480(14)	56(10)	127(10)	145(12)
O(2)	560(15)	395(11)	446(14)	−124(11)	−172(10)	231(12)
O(3)	374(12)	302(9)	392(12)	−47(8)	38(8)	180(10)
O(4)	306(12)	676(15)	359(13)	2(11)	193(11)	−18(10)
O(5)	230(9)	369(10)	324(11)	−61(8)	7(8)	139(9)
O(6)	326(11)	335(10)	297(10)	−19(8)	−21(8)	167(9)

Tables 1 and 2 give the final atomic parameters with standard deviations from least squares. The oxygen atoms are numbered in an order different from that published earlier,[1] and have now numbers in accordance with those in the telluropentathionates described in Refs. 8 and 10.

As seen from Table 2 there is an extremely high value of U_{22} for K(1) compared to all other thermal parameters. This agrees with what was found by the refinement of the two-dimensional film data through difference maps. In the $hk0$ zone the value of B in Å^2 was $2.5+10.0\cos^2\phi$ for K(1), where ϕ is the angle between the normal of the reflecting plane and the direction of maximum vibration of the atom; this direction being parallel to the b axis.[1]

The observed structure factors and those calculated from the final atomic parameters are listed in Table 3.

Table 3. Observed and calculated structure factors ($\times 10$) for potassium barium hexathionate. A minus sign on $F(O)$ indicates an unobserved reflection.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
3	0	0	1361	1367	-9	0	8	185	190	5	1	2	654	-679	-8	1	6	799	-822	-11	1	11	187	201
4	0	0	246	274	-8	0	8	369	366	6	1	2	274	-272	-7	1	6	506	-522	-10	1	11	-57	25
5	0	0	286	321	-7	0	8	620	628	7	1	2	575	-585	-6	1	6	235	-253	-9	1	11	137	-137
6	0	0	710	739	-6	0	8	513	529	8	1	2	93	-87	-5	1	6	416	-415	-8	1	11	102	-102
7	0	0	725	641	-5	0	8	152	164	9	1	2	633	-632	-4	1	6	136	-139	-7	1	11	72	71
8	0	0	1835	1781	-4	0	8	889	875	10	1	2	419	-431	-3	1	6	856	-865	-6	1	11	228	222
9	0	0	760	749	-3	0	8	849	849	11	1	2	262	-266	-2	1	6	81	-86	-5	1	11	-54	-13
10	0	0	-120	4	-2	0	8	1109	1143	12	1	2	223	-207	-1	1	6	621	-625	-4	1	11	-55	-6
11	0	0	130	156	-1	0	8	566	580	13	1	2	364	-361	0	1	6	924	-937	-3	1	11	272	262
12	0	0	887	878	0	0	8	-75	-11	-15	1	3	-59	54	1	1	6	620	-634	-2	1	11	98	-105
13	0	0	215	181	1	0	8	673	681	-14	1	3	115	-110	2	1	6	61	40	-1	1	11	114	-125
14	0	0	296	282	2	0	8	740	739	-13	1	3	249	-254	3	1	6	542	-535	0	1	11	-51	54
-14	0	2	461	-451	3	0	8	-55	-25	-12	1	3	228	223	4	1	6	380	-382	-7	1	12	346	350
-13	0	2	158	-159	4	0	8	689	703	-11	1	3	141	142	5	1	6	292	-289	-6	1	12	158	152
-12	0	2	533	-534	5	0	8	461	460	-10	1	3	52	-57	6	1	6	264	-262	-5	1	12	149	148
-11	0	2	1219	-1213	6	0	8	536	535	-9	1	3	438	448	7	1	6	417	-418	0	2	0	443	403
-10	0	2	360	-368	-12	0	10	308	-304	-8	1	3	592	594	8	1	6	248	-246	1	2	0	535	511
-9	0	2	753	-754	-11	0	10	172	-169	-7	1	3	-44	-18	9	1	6	474	-468	2	2	0	1698	1650
-8	0	2	61	25	-10	0	10	454	-451	-6	1	3	697	-693	-14	1	7	-56	-28	3	2	0	1206	1214
-7	0	2	693	-707	-9	0	10	446	-467	-5	1	3	137	158	-13	1	7	326	333	4	2	0	1575	1603
-6	0	2	1793	-1683	-8	0	10	251	-254	-4	1	3	213	223	-12	1	7	-54	-10	5	2	0	933	939
-5	0	2	1036	-1035	-7	0	10	506	-502	-3	1	3	123	149	-11	1	7	-54	-10	6	2	0	1008	1020
-4	0	2	747	-780	-6	0	10	532	-530	-2	1	3	244	236	-10	1	7	396	404	7	2	0	349	355
-3	0	2	2660	-2815	-5	0	10	776	-771	-1	1	3	74	-84	-9	1	7	96	-88	8	2	0	762	772
-2	0	2	1188	-1213	-4	0	10	169	-177	0	1	3	896	905	-8	1	7	330	-340	9	2	0	318	328
-1	0	2	522	516	-3	0	10	294	-299	1	1	3	-42	-44	-7	1	7	231	-223	10	2	0	692	701
0	0	2	206	204	-2	0	10	511	-528	2	1	3	691	-701	-6	1	7	-47	-8	11	2	0	653	643
1	0	2	2130	-2158	-1	0	10	560	-568	3	1	3	261	269	-5	1	7	761	751	12	2	0	353	350
2	0	2	1215	-1247	0	0	10	467	-482	4	1	3	590	589	-4	1	7	372	374	13	2	0	217	224
3	0	2	2233	-2238	1	0	10	353	-366	5	1	3	438	429	-3	1	7	-44	-17	14	2	0	323	317
4	0	2	727	-711	2	0	10	363	-366	6	1	3	230	-239	-2	1	7	248	241	-14	2	1	-56	18
5	0	2	1218	-1237	3	0	10	511	-506	7	1	3	140	140	-1	1	7	299	301	-13	2	1	168	-171
6	0	2	1163	-1166	-7	0	12	239	222	8	1	3	152	152	0	1	7	458	-469	-12	2	1	94	-89
7	0	2	199	184	-6	0	12	245	238	9	1	3	226	-221	1	1	7	413	-415	-11	2	1	199	195
8	0	2	59	-77	-5	0	12	251	253	10	1	3	-57	65	2	1	7	520	531	-10	2	1	354	-357
9	0	2	1056	-1071	-4	0	12	568	553	11	1	3	155	-27	3	1	7	206	211	-9	2	1	168	-162
10	0	2	553	-537	1	1	0	942	849	12	1	3	182	191	4	1	7	76	75	-8	2	1	185	182
11	0	2	528	-507	2	1	0	537	526	-15	1	4	87	80	5	1	7	61	67	-7	2	1	67	-61
12	0	2	132	-141	3	1	0	111	-91	-14	1	4	370	381	6	1	7	205	-203	-6	2	1	873	858
13	0	2	474	-465	4	1	0	1464	1525	-13	1	4	330	334	7	1	7	217	203	-5	2	1	344	-349
-15	0	4	149	132	5	1	0	214	227	-12	1	4	410	407	8	1	7	-58	-40	-4	2	1	876	-864
-14	0	4	527	515	6	1	0	482	480	-11	1	4	282	300	-14	1	8	431	430	-3	2	1	973	965
-13	0	4	396	400	7	1	0	566	574	-10	1	4	540	549	-13	1	8	273	275	-2	2	1	1157	-1120
-12	0	4	89	81	8	1	0	913	929	-9	1	4	377	377	-12	1	8	328	339	-1	2	1	593	-553
-11	0	4	308	315	9	1	0	193	193	-8	1	4	526	533	-11	1	8	234	243	0	2	1	847	800
-10	0	4	1078	1080	10	1	0	273	271	-7	1	4	184	187	-10	1	8	481	483	1	2	1	169	150
-9	0	4	863	866	11	1	0	361	353	-6	1	4	680	688	-9	1	8	245	246	2	2	1	470	462
-8	0	4	1171	1179	12	1	0	436	427	-5	1	4	806	835	-8	1	8	179	182	3	2	1	74	-85
-7	0	4	226	236	13	1	0	199	199	-4	1	4	778	786	-7	1	8	328	329	4	2	1	174	-171
-6	0	4	1114	1150	14	1	0	272	265	-3	1	4	388	372	-6	1	8	739	744	5	2	1	63	-23
-5	0	4	1118	1127	-14	1	1	118	-107	-2	1	4	1361	1348	-5	1	8	447	454	6	2	1	-43	-15
-4	0	4	194	209	-13	1	1	220	-225	-1	1	4	317	-285	-4	1	8	329	332	7	2	1	304	-304
-3	0	4	501	505	-12	1	1	208	-213	0	1	4	566	577	-3	1	8	404	406	8	2	1	-48	24
-2	0	4	1529	1897	-11	1	1	-52	42	1	1	4	409	428	-2	1	8	614	618	9	2	1	413	418
-1	0	4	1481	1564	-10	1	1	144	136	2	1	4	207	220	-1	1	8	58	54	10	2	1	268	-268
0	0	4	745	763	-9	1	1	369	-368	3	1	4	852	872	0	1	8	415	416	11	2	1	182	-198
1	0	4	123	126	-8	1	1	56	55	4	1	4	680	681	1	1	8	222	228	12	2	1	96	98
2	0	4	1560	1571	-7	1	1	695	696	5	1	4	108	93	2	1	8	535	547	13	2	1	82	-80
3	0	4	487	497	-6	1	1	1159	-1181	6	1	4	942	955	3	1	8	350	350	-14	2	2	341	-328
4	0	4	980	987	-5	1	1	782	-787	7	1	4	148	150	4	1	8	148	141	-13	2	2	632	-641
5	0	4	578	579	-4	1	1	699	724	8	1	4	334	324	5	1	8	305	310	-12	2	2	194	-203
6	0	4	848	856	-3	1	1	273	266	9	1	4	253	248	6	1	8	430	427	-11	2	2	146	-146
7	0	4	1017	1008	-2	1	1	899	878	10	1	4	315	322	-13	1	9	-58	-35	-10	2	2	468	-469
8	0	4	237	224	-1	1	1	532	-503	11	1	4	279	274	-12	1	9	-57	-26	9	2	2	730	-724
9	0	4	64	-60	0	1	1	491	-461	-15	1	5	104	-97	-11	1	9	177	176	-8	2	2	542	-554
10	0	4	560	553	1	1	1	180	187	-14	1	5	294	-292	-10	1	9	-54	27	-7	2	2	1187	-1194
11	0	4	315	309	2	1	1	1452	-1469	-13	1	5	82	79	-9	1	9	208	-219	-6	2	2	806	-834
-15	0	6	347	-335	3	1	1	1416	-1444	-12	1	5	213	229	-8	1	9	269	-274	-5	2	2	1386	-1356
-14	0	6	222	-226	4	1	1	61	43	-11	1	5	236	-243	-7	1	9	264	-266	-4	2	2	860	-835
-13	0	6	618	-616	5	1	1	1063	1083	-10	1	5	68	61	-6	1	9	218	210	-3	2	2	980	-982
-12	0	6	570	-568	6	1	1	148	-120	-9	1	5	331	343	-5	1	9	229	239	-2	2	2	497	-496
-11	0	6	381	-400	7	1	1	334	-343	-8	1	5	241	-244	-4	1	9	213	-211	-1	2	2	2340	-2421
-10	0	6	82	-59	8	1	1	323	327	-7	1	5	793	-802	-3	1	9	122	124	0	2	2	1347	-1351
-9	0	6	241	-252	9	1	1	243	-243	-6	1	5	475	-468	-2	1	9	73	-82	1	2	2	456	-467
-8	0	6	961	-984	10	1	1	175	-171	-5	1	5	334	342	-1	1	9	338	-343	2	2	2	1041	-1052
-7	0	6	1451	-1487	11	1	1	118	-115	-4	1	5	181	-178	0	1	9	334	-347	3	2	2	1022	-1009
-6	0	6	85	65	12	1	1	60	-43	-3	1	5	-42	21	1	1	9	100	-89	4	2	2	-43	-41
-5	0	6	1449	-1463	13	1	1	207	203	-2	1	5	86	-89	2	1	9	275	274	5	2	2	1139	-1165
-4	0	6	1637	-1673	-14	1	2	295	-295	-1	1	5	63	44	3	1	9	-58	60	6	2	2	625	-630
-3	0	6	-82	-9	-13	1	2	478	-473	0	1	5	503	494	4	1	9	-58	-34	7	2	2	933	-933
-2	0	6	231	-238	-12	1	2	-55	-62	1	1	5	926	-933	5	1	9	97	-88	8	2	2	796	-791
-1	0	6	868	-890	-11	1	2	577	-587	2	1	5	296	-299	-12	1	10	264	-267	9	2	2	494	-490
0	0	6	876	-873	-10	1	2	596	-593	3	1	5	686	695	-11	1	10	295	-298	10	2	2	136	-133
1	0	6	1261	-1252	-9	1	2	293	-295	4	1	5	210	-216	-10	1	10	306	-305	11	2	2	544	-542
2	0	6	146	-116	-8	1	2	439	-453	5	1	5	240	-238	-9	1	10	485	-481	12	2	2	220	-210
3	0	6	634	-633	-7	1	2	627	-649	6	1	5	167	-157	-8	1	10	192	-200	-15	2	3	109	101
4	0	6	748	-762	-6	1	2	242	-246	7	1	5	118	-118	-7	1	10	274	-271	-14	2	3	-56	-35
5	0	6	566	-560	-5	1	2	1296	-1298	8	1	5	85	-87	-6	1	10	238	-236	-13	2	3	76	75
6	0	6	131	121	-4	1	2	314	300	9	1	5	100	-102	-5	1	10	325	-320	-12	2	3	64	-73
7	0	6	671	-681	-3	1	2	763	-790	10	1	5	-57	-40	-4	1	10	399	-397	-11	2	3	54	43
8	0	6	844	-829	-2	1	2	975	-984	-15	1	6	400	-408	-3	1	10	290	-299	-10	2	3	157	-159
9	0	6	336	-323	-1	1	2	664	-663	-14	1	6	146	-135	-2	1	10	215	-215	-9	2	3	-47	0
-14	0	8	345	351	0	1	2	333	-325	-13	1	6	249	-256	-1	1	10	554	-549	-8	2	3	356	353
-13	0	8	317	324	1	1	2	1183	-1204	-12	1	6	334	-333	0	1	10	111	-111	-7	2	3	450	451
-12	0	8	209	195	2	1	2	709	-718	-11	1	6	537	-532	1	1	10	265	-260	-6	2	3	324	314
-11	0	8	609	626	3	1	2	846	-832	-10	1	6	65	-74	2	1	10	254	-249	-5	2	3	375	-366
-10	0	8	966	986	4	1	2	186	-207	-9	1	6	535	-544	3	1	10	301	-313	-4	2	3	286	-256

Table 3. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
-3	2	3	498	-479	-2	2	7	137	-155	0	3	1	-41	3	-2	3	5	65	48	-4	3	10	161	-162
-2	2	3	578	-566	-1	2	7	221	221	1	3	1	1019	1007	-1	3	5	279	-295	-3	3	10	400	-400
-1	2	3	355	357	0	2	7	90	84	2	3	1	364	-379	0	3	5	63	52	-2	3	10	281	-282
0	2	3	116	-114	1	2	7	165	-161	3	3	1	361	-353	1	3	5	229	-231	-1	3	10	310	-302
1	2	3	750	767	2	2	7	149	-149	4	3	1	572	-565	2	3	5	873	-874	0	3	10	331	-335
2	2	3	220	217	3	2	7	420	423	5	3	1	876	-870	3	3	5	243	-248	1	3	10	277	-279
3	2	3	403	-396	4	2	7	77	-81	6	3	1	429	-433	4	3	5	318	-333	2	3	10	256	-251
4	2	3	289	283	5	2	7	187	-182	7	3	1	452	-447	5	3	5	432	-430	-10	3	11	129	133
5	2	3	301	-312	6	2	7	269	268	8	3	1	82	-58	6	3	5	-51	38	-9	3	11	84	83
6	2	3	-47	11	7	2	7	-57	26	9	3	1	316	312	7	3	5	217	214	-8	3	11	171	163
7	2	3	188	184	8	2	7	-56	15	10	3	1	110	-108	8	3	5	-53	-12	-7	3	11	129	135
8	2	3	-51	34	-14	2	8	500	503	11	3	1	417	-422	9	3	5	209	-205	-6	3	11	159	150
9	2	3	237	234	-13	2	8	402	405	12	3	1	112	-127	10	3	5	251	-243	-5	3	11	146	135
10	2	3	206	-199	-12	2	8	458	466	13	3	1	66	-78	-14	3	6	330	-327	-4	3	11	62	-48
11	2	3	-55	-41	-11	2	8	289	281	-14	3	2	266	-277	-13	3	6	475	-469	-3	3	11	240	270
12	2	3	140	134	-10	2	8	360	360	-13	3	2	293	-296	-12	3	6	344	-344	-2	3	11	309	314
-15	2	4	214	219	-9	2	8	412	412	-12	3	2	424	-416	-11	3	6	370	-373	-1	3	11	-61	73
-14	2	4	253	248	-8	2	8	612	615	-11	3	2	638	-638	-10	3	6	346	-335	0	4	0	752	758
-13	2	4	454	454	-7	2	8	502	507	-10	3	2	-51	30	-9	3	6	443	-449	1	4	0	1144	1139
-12	2	4	793	753	-6	2	8	909	900	-9	3	2	581	-579	-8	3	6	212	-202	2	4	0	1281	1253
-11	2	4	438	444	-5	2	8	912	897	-8	3	2	287	-285	-7	3	6	622	-630	3	4	0	423	426
-10	2	4	694	714	-4	2	8	367	362	-7	3	2	542	-550	-6	3	6	220	-211	4	4	0	661	648
-9	2	4	442	447	-3	2	8	-48	9	-6	3	2	743	-740	-5	3	6	949	-931	5	4	0	170	180
-8	2	4	328	327	-2	2	8	656	657	-5	3	2	914	-901	-4	3	6	658	-669	6	4	0	1349	1346
-7	2	4	664	669	-1	2	8	291	287	-4	3	2	724	-718	-3	3	6	219	-218	7	4	0	552	554
-6	2	4	841	856	0	2	8	694	698	-3	3	2	928	-909	-2	3	6	478	-479	8	4	0	300	298
-5	2	4	238	258	1	2	8	728	746	-2	3	2	551	-550	-1	3	6	445	-452	9	4	0	584	582
-4	2	4	1774	1746	2	2	8	642	646	-1	3	2	293	-285	0	3	6	296	-304	10	4	0	461	455
-3	2	4	1172	1154	3	2	8	486	480	0	3	2	71	-78	1	3	6	701	-703	11	4	0	188	176
-2	2	4	856	832	4	2	8	407	406	1	3	2	1616	-1603	2	3	6	297	-300	12	4	0	328	317
-1	2	4	778	767	5	2	8	73	48	2	3	2	101	-108	3	3	6	748	-743	13	4	0	263	268
0	2	4	1390	1354	6	2	8	356	361	3	3	2	1077	-1080	4	3	6	213	-214	-14	4	1	-58	-45
1	2	4	719	723	-13	2	9	-59	70	4	3	2	544	-543	5	3	6	411	-415	-13	4	1	211	-211
2	2	4	1112	1132	-12	2	9	113	-114	5	3	2	274	-282	6	3	6	193	-190	-12	4	1	97	-99
3	2	4	713	710	-11	2	9	145	-140	6	3	2	541	-553	7	3	6	314	-315	-11	4	1	92	89
4	2	4	557	556	-10	2	9	100	75	7	3	2	424	-418	8	3	6	299	-304	-10	4	1	166	-160
5	2	4	571	579	-9	2	9	97	92	8	3	2	301	-298	9	3	6	247	-242	-9	4	1	192	-180
6	2	4	540	544	-8	2	9	164	-163	9	3	2	579	-591	-14	3	7	-58	43	-8	4	1	82	-75
7	2	4	-30	16	-7	2	9	-52	0	10	3	2	322	-320	-13	3	7	214	211	-7	4	1	390	390
8	2	4	794	759	-6	2	9	100	-95	11	3	2	474	-468	-12	3	7	149	142	-6	4	1	197	-206
9	2	4	487	480	-5	2	9	156	163	12	3	2	145	-136	-11	3	7	-54	-31	-5	4	1	563	-560
10	2	4	456	435	-4	2	9	-51	31	-14	3	3	-55	35	-10	3	7	112	83	-4	4	1	56	53
11	2	4	377	369	-3	2	9	313	-319	-13	3	3	304	314	-9	3	7	575	591	-3	4	1	349	348
-15	2	5	133	-119	-2	2	9	190	192	-12	3	3	342	339	-8	3	7	428	425	-2	4	1	524	-506
-14	2	5	75	-89	-1	2	9	-52	1	-11	3	3	140	-148	-7	3	7	-48	2	-1	4	1	992	-954
-13	2	5	62	71	0	2	9	270	-270	-10	3	3	-51	57	-6	3	7	51	30	0	4	1	520	505
-12	2	5	60	-84	1	2	9	67	61	-9	3	3	87	100	-5	3	7	266	259	1	4	1	477	449
-11	2	5	133	-139	2	2	9	124	-113	-8	3	3	192	-188	-4	3	7	-47	-12	2	4	1	72	52
-10	2	5	266	-263	3	2	9	153	158	-7	3	3	801	797	-3	3	7	-45	13	3	4	1	-41	1
-9	2	5	160	164	4	2	9	-57	-37	-6	3	3	579	573	-2	3	7	313	314	4	4	1	352	-339
-8	2	5	221	219	5	2	9	124	-110	-5	3	3	141	-147	-1	3	7	770	772	5	4	1	636	631
-7	2	5	102	108	-12	2	10	271	-258	-4	3	3	690	692	0	3	7	408	407	6	4	1	285	-292
-6	2	5	178	-113	-11	2	10	549	-559	-3	3	3	550	541	1	3	7	-50	48	7	4	1	837	-843
-5	2	5	110	-119	-10	2	10	363	-371	-2	3	3	134	-163	2	3	7	-50	47	8	4	1	259	257
-4	2	5	140	145	-9	2	10	469	-456	-1	3	3	1254	1228	3	3	7	151	150	9	4	1	88	-63
-3	2	5	707	-655	-8	2	10	502	-507	0	3	3	787	786	4	3	7	90	102	10	4	1	190	-194
-2	2	5	231	-243	-7	2	10	298	-304	1	3	3	197	195	5	3	7	-54	49	11	4	1	-54	-26
-1	2	5	637	617	-6	2	10	180	-173	2	3	3	813	813	6	3	7	204	201	12	4	1	-56	-33
0	2	5	247	-252	-5	2	10	550	-579	3	3	3	273	-253	7	3	7	451	454	13	4	1	-56	22
1	2	5	311	315	-4	2	10	535	-533	4	3	3	527	-525	-14	3	8	174	168	-14	4	2	62	-46
2	2	5	-46	-16	-3	2	10	604	-605	5	3	3	505	513	-13	3	8	280	277	-13	4	2	442	-441
3	2	5	169	-171	-2	2	10	505	-500	6	3	3	-48	11	-12	3	8	334	331	-12	4	2	470	-474
4	2	5	190	185	-1	2	10	351	-351	7	3	3	210	213	-11	3	8	311	309	-11	4	2	593	-604
5	2	5	322	-324	0	2	10	161	-150	8	3	3	833	838	-10	3	8	415	420	-10	4	2	419	-426
6	2	5	74	-66	1	2	10	412	-412	9	3	3	160	171	-9	3	8	318	319	-9	4	2	603	-612
7	2	5	188	185	2	2	10	139	-129	10	3	3	-54	-10	-8	3	8	528	535	-8	4	2	710	-711
8	2	5	-53	28	3	2	10	406	-406	11	3	3	121	106	-7	3	8	387	388	-7	4	2	291	-289
9	2	5	149	-147	-10	2	11	138	131	12	3	3	71	-31	-6	3	8	423	429	-6	4	2	158	-168
10	2	5	135	-149	-9	2	11	-58	11	-14	3	4	392	381	-5	3	8	105	99	-5	4	2	1284	-1272
-15	2	6	511	-497	-8	2	11	116	-121	-13	3	4	160	162	-4	3	8	672	661	-4	4	2	422	-428
-14	2	6	176	-187	-7	2	11	153	153	-12	3	4	210	208	-3	3	8	372	371	-3	4	2	993	-982
-13	2	6	285	-282	-6	2	11	-56	45	-11	3	4	454	449	-2	3	8	262	265	-2	4	2	471	-469
-12	2	6	351	-352	-5	2	11	-56	-37	-10	3	4	629	632	-1	3	8	495	499	-1	4	2	733	-713
-11	2	6	548	-559	-4	2	11	-54	-19	-9	3	4	306	310	0	3	8	335	342	0	4	2	1098	-1095
-10	2	6	606	-615	-3	2	11	-55	34	-8	3	4	939	936	1	3	8	292	296	1	4	2	1053	-1016
-9	2	6	823	-830	-2	2	11	140	126	-7	3	4	184	158	2	3	8	472	469	2	4	2	631	-636
-8	2	6	568	-578	-1	2	11	-56	-35	-6	3	4	536	546	3	3	8	152	156	3	4	2	1348	-1338
-7	2	6	713	-705	0	2	11	94	-94	-5	3	4	395	403	4	3	8	532	532	4	4	2	931	-929
-6	2	6	438	-440	0	3	0	2075	2005	-4	3	4	59	56	5	3	8	191	183	5	4	2	397	-405
-5	2	6	418	-421	1	3	0	103	-59	-3	3	4	686	691	6	3	8	311	309	6	4	2	-68	-23
-4	2	6	393	-395	2	3	0	773	782	-2	3	4	1253	1240	-13	3	9	-56	37	7	4	2	748	-753
-3	2	6	1215	-1219	3	3	0	732	725	-1	3	4	752	757	-12	3	9	190	-188	8	4	2	213	-210
-2	2	6	834	-834	4	3	0	529	533	0	3	4	884	877	-11	3	9	308	-304	9	4	2	467	-469
-1	2	6	1021	-1014	5	3	0	698	713	1	3	4	289	292	-10	3	9	59	-54	10	4	2	441	-439
0	2	6	592	-599	6	3	0	644	644	2	3	4	675	680	-9	3	9	84	65	11	4	2	375	-380
1	2	6	678	-685	7	3	0	396	407	3	3	4	90	-64	-8	3	9	299	-301	12	4	2	426	-416
2	2	6	379	-378	8	3	0	661	665	4	3	4	733	743	-7	3	9	225	-233	-14	4	3	66	60
3	2	6	607	-616	9	3	0	343	336	5	3	4	363	356	-6	3	9	203	-198	-13	4	3	-57	-60
4	2	6	560	-564	10	3	0	504	505	6	3	4	463	471	-5	3	9	336	-330	-12	4	3	159	156
5	2	6	667	-678	11	3	0	81	78	7	3	4	591	594	-4	3	9	234	-231	-11	4	3	186	194
6	2	6	529	-529	12	3	0	432	428	8	3	4	245	242	-3	3	9	150	-141	-10	4	3	92	-89
7	2	6	477	-464	13	3	0	241	229	9	3	4	235	232	-2	3	9	158	-154	-9	4	3	198	196
8	2	6	104	-101	-14	3	1	-55	-1	10	3	4	351	359	-1	3	9	279	284	-8	4	3	340	337
9	2	6	351	-353	-13	3	1	117	-101	11	3	4	90	67	0	3	9	162	-154	-7	4	3	84	-78
-14	2	7	-55	32	-12	3	1	-55	25	-14	3	5	85	-75	1	3	9	416	-428	-6	4	3	523	-519
-13	2	7	75	72	-11	3	1	-52	38	-13	3	5	-54	6	2	3	9	83	-87	-5	4	3	499	513
-12	2	7	132	129	-10	3	1	364	-369	-12	3	5	333	-333	3	3	9	190	-186	-4	4	3	175	174
-11	2	7	128	-115	-9	3	1	652	-647	-11	3	5	210	-215	4	3	9	327	-338	-3	4	3	-42	11
-10	2	7	249	-259	-8	3	1	338	-340	-10	3	5	435	-435	-12	3	10	192	-196	-2	4	3	456	444
-9	2	7	513	511	-7	3	1	-46	-26	-9	3	5	258	-253	-11	3	10	234	-228	-1	4	3	372	-363
-8	2	7	-51	34	-6	3	1	85	-102	-8	3	5	368	369	-10	3	10	356	-344	0	4	3	179	198
-7	2	7	271	-271	-5	3	1	70	-70	-7	3	5	315	-325	-9	3	10	282	-285	1	4	3	286	282
-6	2	7	226	222	-4	3	1	875	-859	-6	3	5	534	-541	-8	3	10	217	-208	2	4	3	628	-626
-5	2	7	111	118	-3	3	1	546	-544	-5	3	5	244	240	-7	3	10	551	-549	3	4	3	159	157
-4	2	7	-47	50	-2	3	1	462	-453	-4	3	5	817	-808	-6	3	10	305	-309	4	4	3	594	603
-3	2	7	115	-110	-1	3	1	1613	-1584	-3	3	5	581	-574	-5	3	10	331	-321	5	4	3	66	53

Table 3. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
6	4	2	185	-188	-7	4	8	271	270	-2	5	2	-42	-38	2	5	6	590	-593	-3	6	1	455	-439
7	4	3	228	237	-6	4	8	131	129	-1	5	2	1938	-1922	3	5	6	343	-342	-2	6	1	104	94
8	4	3	-53	-44	-5	4	8	435	424	0	5	2	962	-950	4	5	6	125	-126	-1	6	1	117	-133
9	4	3	-53	-16	-4	4	8	840	837	1	5	2	252	220	5	5	6	556	-561	0	6	1	-43	-43
10	4	3	211	208	-3	4	8	524	536	2	5	2	273	-285	6	5	6	642	-636	1	6	1	499	-499
11	4	3	97	-76	-2	4	8	567	565	3	5	2	762	-766	7	5	6	395	-375	2	6	1	262	-262
-14	4	4	421	424	-1	4	8	513	504	4	5	2	570	-574	8	5	6	64	61	3	6	1	509	509
-13	4	4	-56	30	0	4	8	635	635	5	5	2	823	-818	-13	5	7	154	157	4	6	1	743	-744
-12	4	4	284	284	1	4	8	60	-59	6	5	2	282	-297	-12	5	7	198	195	5	6	1	867	-862
-11	4	4	414	419	2	4	8	217	216	7	5	2	851	-856	-11	5	7	388	381	6	6	1	327	325
-10	4	4	422	420	3	4	8	425	413	8	5	2	655	-653	-10	5	7	215	208	7	6	1	66	68
-9	4	4	352	354	4	4	8	457	444	9	5	2	-53	17	-9	5	7	225	219	8	6	1	141	-133
-8	4	4	908	952	5	4	8	409	419	10	5	2	136	135	-8	5	7	94	84	9	6	1	62	-59
-7	4	4	905	855	6	4	8	251	244	11	5	2	531	-533	-7	5	7	300	296	10	6	1	65	-46
-6	4	4	526	512	-12	4	9	87	-97	12	5	2	270	-268	-6	5	7	84	96	11	6	1	97	-96
-5	4	4	501	492	-11	4	9	96	86	-14	5	3	138	132	-5	5	7	334	334	12	6	1	262	-262
-4	4	4	793	751	-10	4	9	58	-37	-13	5	3	74	82	-4	5	7	781	777	-13	6	2	260	-261
-3	4	4	375	379	-9	4	9	240	-240	-12	5	3	-52	7	-3	5	7	376	380	-12	6	2	147	-139
-2	4	4	1294	1292	-8	4	9	129	-115	-11	5	3	389	385	-2	5	7	353	358	-11	6	2	312	-311
-1	4	4	181	183	-7	4	9	141	-129	-10	5	3	376	371	-1	5	7	325	326	-10	6	2	207	-204
0	4	4	710	730	-6	4	9	70	-79	-9	5	3	562	564	0	5	7	145	-143	-9	6	2	492	-496
1	4	4	519	536	-5	4	9	228	236	-8	5	3	229	236	1	5	7	409	399	-8	6	2	544	-535
2	4	4	123	117	-4	4	9	248	-255	-7	5	3	212	217	2	5	7	180	186	-7	6	2	763	-754
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8	4	4	444	458	2	4	9	-54	19	-1	5	3	859	869	-13	5	8	294	283	-1	6	2	1147	-1111
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-5	4	5	232	236	-2	4	10	140	-139	11	5	3	214	223	-1	5	8	518	522	11	6	2	283	-285
-4	4	5	118	123	-1	4	10	443	-439	-14	5	4	141	143	0	5	8	645	648	-13	6	3	283	278
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0	4	5	145	-136	-9	4	11	84	-89	-10	5	4	253	242	4	5	8	447	450	-9	6	3	105	95
1	4	5	820	-817	-8	4	11	-57	-39	-9	5	4	183	179	5	5	8	-56	-52	-8	6	3	214	-201
2	4	5	107	-107	-7	4	11	238	225	-8	5	4	389	380	-12	5	9	-56	-17	-7	6	3	572	566
3	4	5	330	326	-6	4	11	218	212	-7	5	4	887	890	-11	5	9	106	-91	-6	6	3	669	663
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9	4	5	237	-233	0	5	0	-82	-39	-1	5	4	187	203	-5	5	9	136	-137	0	6	3	-67	15
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-9	4	6	327	-326	6	5	0	914	909	5	5	4	648	644	1	5	9	109	-107	6	6	3	375	378
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-7	4	6	487	-456	8	5	0	181	177	7	5	4	91	-74	3	5	9	-54	14	8	6	3	223	216
-6	4	6	890	-893	9	5	0	257	271	8	5	4	687	697	-11	5	10	512	-510	9	6	3	110	112
-5	4	6	1012	-1009	10	5	0	878	880	9	5	4	430	433	-10	5	10	173	-164	10	6	3	250	254
-4	4	6	313	-312	11	5	0	511	506	10	5	4	344	336	-9	5	10	129	-120	11	6	3	-59	46
-3	4	6	547	-547	12	5	0	81	75	-14	5	5	214	-215	-8	5	10	398	-392	-13	6	4	311	313
-2	4	6	425	-420	13	5	0	278	275	-13	5	5	275	-267	-7	5	10	328	-320	-12	6	4	412	412
-1	4	6	706	-703	-13	5	1	69	-54	-12	5	5	203	-209	-6	5	10	121	-113	-11	6	4	323	332
0	4	6	113	-124	-12	5	1	533	-527	-11	5	5	55	27	-5	5	10	391	-384	-10	6	4	304	308
1	4	6	711	-705	-11	5	1	149	-153	-10	5	5	242	-234	-4	5	10	389	-376	-9	6	4	-52	-44
2	4	6	920	-928	-10	5	1	117	-111	-9	5	5	-53	-47	-3	5	10	539	-528	-8	6	4	397	401
3	4	6	518	-500	-9	5	1	361	-374	-8	5	5	509	-506	-2	5	10	270	-264	-7	6	4	213	209
4	4	6	205	-204	-8	5	1	159	-154	-7	5	5	648	-645	-1	5	10	81	-95	-6	6	4	701	699
5	4	6	311	-303	-7	5	1	483	-473	-6	5	5	343	-333	0	5	10	232	-216	-5	6	4	838	819
6	4	6	279	-281	-6	5	1	375	-377	-5	5	5	623	-624	1	5	10	444	-445	-4	6	4	504	506
7	4	6	501	-497	-5	5	1	304	-299	-4	5	5	433	-424	-8	5	11	102	97	-3	6	4	504	509
8	4	6	141	-144	-4	5	1	593	-586	-3	5	5	-44	15	-7	5	11	183	174	-2	6	4	264	268
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-10	4	7	290	301	1	5	1	805	-800	2	5	5	519	-521	-2	5	11	76	67	3	6	4	443	449
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-8	4	7	99	-95	3	5	1	938	-945	4	5	5	190	-194	1	6	0	201	205	5	6	4	52	43
-7	4	7	209	-206	4	5	1	108	-117	5	5	5	389	-401	2	6	0	1004	997	6	6	4	180	180
-6	4	7	64	49	5	5	1	315	-318	6	5	5	-53	46	3	6	0	244	243	7	6	4	302	298
-5	4	7	310	309	6	5	1	386	-392	7	5	5	467	-462	4	6	0	936	933	8	6	4	286	286
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-3	4	7	124	116	8	5	1	436	-436	9	5	5	-57	14	6	6	0	266	270	10	6	4	282	291
-2	4	7	59	42	9	5	1	357	-354	-14	5	6	290	-286	7	6	0	483	486	-13	6	5	81	-81
-1	4	7	281	289	10	5	1	202	-204	-13	5	6	265	-269	8	6	0	144	138	-12	6	5	398	-399
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2	4	7	345	351	-14	5	2	98	-87	-10	5	6	687	-676	11	6	0	94	97	-9	6	5	620	-608
3	4	7	375	370	-13	5	2	413	-415	-9	5	6	605	-600	12	6	0	248	251	-8	6	5	-50	-22
4	4	7	93	-75	-12	5	2	346	-335	-8	5	6	84	79	-13	6	1	-56	37	-7	6	5	331	315
5	4	7	1139	148	-11	5	2	-56	-16	-7	5	6	565	-554	-12	6	1	-57	-19	-6	6	5	245	-244
6	4	7	-53	1	-10	5	2	310	-308	-6	5	6	821	-820	-11	6	1	422	-416	-5	6	5	248	-246
7	4	7	95	75	-9	5	2	939	-938	-5	5	6	389	-392	-10	6	1	220	-222	-4	6	5	642	-634
-13	4	8	257	259	-8	5	2	582	-582	-4	5	6	64	-67	-9	6	1	69	71	-3	6	5	136	-130
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-9	4	8	442	442	-4	5	2	916	-909	0	5	6	167	160	-5	6	1	465	444	1	6	5	474	470
-8	4	8	552	544	-3	5	2	382	-381	1	5	6	310	-317	-4	6	1	581	-576	2	6	5	-49	-4

Table 3. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
3	6	5	616	-626	-11	7	1	236	-241	-2	7	5	520	-517	-5	8	1	393	-386	-9	8	6	135	-136
4	6	5	474	-469	-10	7	1	424	-418	-1	7	5	488	-485	-4	8	1	115	-106	-8	8	6	84	-65
5	6	5	-54	58	-9	7	1	62	-58	0	7	5	405	-395	-3	8	1	304	-300	-7	8	6	276	-264
6	6	5	134	-137	-8	7	1	300	-309	1	7	5	166	-158	-2	8	1	60	-15	-6	8	6	344	-354
7	6	5	123	-129	-7	7	1	479	-472	2	7	5	183	-176	-1	8	1	436	425	-5	8	6	361	-359
8	6	5	-57	-32	-6	7	1	322	-326	3	7	5	456	-459	0	8	1	682	-674	-4	8	6	244	-239
9	6	5	-56	-37	-5	7	1	296	-292	4	7	5	397	-391	1	8	1	562	-557	-3	8	6	531	-537
-13	6	6	205	-187	-4	7	1	600	-594	5	7	5	188	-183	2	8	1	310	-315	-2	8	6	142	-135
-12	6	6	215	-221	-3	7	1	777	-761	6	7	5	296	-293	3	8	1	616	-632	-1	8	6	-49	1
-11	6	6	316	-321	-2	7	1	627	-622	7	7	5	143	-145	4	8	1	169	162	0	8	6	198	-193
-10	6	6	353	-357	-1	7	1	511	-506	8	7	5	251	-259	5	8	1	180	-169	1	8	6	241	-241
-9	6	6	739	-745	0	7	1	267	-264	-13	7	6	519	-503	6	8	1	232	-231	2	8	6	194	-176
-8	6	6	190	-187	1	7	1	455	-465	-12	7	6	270	-271	7	8	1	57	45	3	8	6	354	-357
-7	6	6	216	-226	2	7	1	291	-298	-11	7	6	428	-425	8	8	1	488	-482	4	8	6	158	-171
-6	6	6	334	-329	3	7	1	131	-144	-10	7	6	277	-279	9	8	1	425	-423	5	8	6	206	-195
-5	6	6	296	-296	4	7	1	686	-690	-9	7	6	166	-161	10	8	1	167	-185	6	8	6	186	-182
-4	6	6	58	-52	5	7	1	437	-437	-8	7	6	317	-310	11	8	1	-57	-43	-11	8	7	396	384
-3	6	6	582	-573	6	7	1	379	-373	-7	7	6	421	-421	-12	8	2	134	-129	-10	8	7	305	308
-2	6	6	657	-657	7	7	1	340	-339	-6	7	6	347	-336	-11	8	2	290	-291	-9	8	7	-55	33
-1	6	6	418	-433	8	7	1	249	-252	-5	7	6	676	-674	-10	8	2	301	-296	-8	8	7	69	-63
0	6	6	436	-448	9	7	1	415	-424	-4	7	6	718	-709	-9	8	2	225	-215	-7	8	7	391	378
1	6	6	309	-314	10	7	1	130	-123	-3	7	6	242	-244	-8	8	2	147	-155	-6	8	7	99	107
2	6	6	159	-160	11	7	1	170	-164	-2	7	6	55	-65	-7	8	2	402	-405	-5	8	7	120	96
3	6	6	625	-614	-13	7	2	153	-147	-1	7	6	685	-674	-6	8	2	161	-147	-4	8	7	467	458
4	6	6	-54	-15	-12	7	2	371	-367	0	7	6	119	-111	-5	8	2	430	-432	-3	8	7	209	203
5	6	6	453	-460	-11	7	2	507	-497	1	7	6	568	-568	-4	8	2	305	-300	-2	8	7	218	230
6	6	6	419	-426	-10	7	2	268	-276	2	7	6	740	-734	-3	8	2	129	-133	-1	8	7	97	109
7	6	6	105	-100	-9	7	2	260	-259	3	7	6	217	-219	-2	8	2	316	-319	0	8	7	171	-170
-13	6	7	-60	-7	-8	7	2	253	-240	4	7	6	513	-510	-1	8	2	284	-293	1	8	7	489	487
-12	6	7	176	173	-7	7	2	390	-395	5	7	6	324	-315	0	8	2	110	-107	2	8	7	257	253
-11	6	7	168	154	-6	7	2	650	-656	6	7	6	100	107	1	8	2	553	-568	3	8	7	110	108
-10	6	7	166	-160	-5	7	2	527	-526	7	7	6	396	-390	2	8	2	276	-276	4	8	7	281	272
-9	6	7	96	81	-4	7	2	436	-438	-12	7	7	114	123	3	8	2	266	-257	5	8	7	193	192
-8	6	7	328	327	-3	7	2	1448	-1454	-11	7	7	315	310	4	8	2	466	-464	-10	8	8	235	233
-7	6	7	284	286	-2	7	2	333	-333	-10	7	7	195	197	5	8	2	217	-223	-9	8	8	306	295
-6	6	7	119	123	-1	7	2	124	-120	-9	7	7	153	153	6	8	2	99	-108	-8	8	8	135	137
-5	6	7	131	-103	0	7	2	625	-627	-8	7	7	323	330	7	8	2	287	-291	-7	8	8	167	167
-4	6	7	-50	23	1	7	2	513	-505	-7	7	7	541	551	8	8	2	118	-119	-6	8	8	353	348
-3	6	7	579	573	2	7	2	650	-654	-6	7	7	377	378	9	8	2	322	-326	-5	8	8	-53	23
-2	6	7	58	-87	3	7	2	547	-542	-5	7	7	259	265	10	8	2	178	-178	-4	8	8	211	205
-1	6	7	-51	0	4	7	2	395	-403	-4	7	7	-51	6	-12	8	3	111	126	-3	8	8	274	260
0	6	7	536	531	5	7	2	762	-776	-3	7	7	416	404	-11	8	3	422	417	-2	8	8	244	254
1	6	7	241	237	6	7	2	207	-203	-2	7	7	232	230	-10	8	3	163	157	-1	8	8	248	233
2	6	7	149	-155	7	7	2	298	-296	-1	7	7	158	150	-9	8	3	383	369	0	8	8	239	233
3	6	7	81	-79	8	7	2	243	-241	0	7	7	447	454	-8	8	3	139	143	1	8	8	75	88
4	6	7	-55	45	9	7	2	491	-492	1	7	7	432	433	-7	8	3	282	-297	2	8	8	236	231
5	6	7	252	257	10	7	2	424	-419	2	7	7	317	321	-6	8	3	207	217	3	8	8	145	125
6	6	7	100	100	11	7	2	169	-165	3	7	7	197	193	-5	8	3	210	205	-9	8	9	216	-207
-12	6	8	375	374	-13	7	3	311	302	4	7	7	150	158	-4	8	3	377	376	-8	8	9	301	-303
-11	6	8	296	259	-12	7	3	140	151	5	7	7	356	349	-3	8	3	762	769	-7	8	9	178	-168
-10	6	8	68	96	-11	7	3	79	78	-11	7	8	317	315	-2	8	3	445	441	-6	8	9	157	-150
-9	6	8	282	282	-10	7	3	235	242	-10	7	8	564	556	-1	8	3	517	520	-5	8	9	150	-168
-8	6	8	506	506	-9	7	3	344	340	-9	7	8	207	206	0	8	3	57	-51	-4	8	9	57	56
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-6	6	8	535	532	-7	7	3	558	557	-7	7	8	502	498	2	8	3	81	73	-2	8	9	254	-248
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2	6	8	341	340	1	7	3	612	613	1	7	8	267	265	-12	8	4	158	155	3	9	0	543	537
3	6	8	224	230	2	7	3	503	503	2	7	8	257	255	-11	8	4	133	126	4	9	0	915	910
4	6	8	287	291	3	7	3	419	414	3	7	8	167	173	-10	8	4	113	116	5	9	0	532	529
5	6	8	144	149	4	7	3	110	108	4	7	8	364	363	-9	8	4	400	399	6	9	0	-67	-35
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-9	6	10	278	-290	-3	7	4	-47	-7	-5	7	10	323	-333	8	8	4	131	130	0	9	1	392	-385
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3	7	0	663	669	-13	7	5	293	-215	8	8	0	331	328	0	8	5	519	-520	-9	9	2	380	-384
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5	7	0	210	159	-11	7	5	345	-357	10	8	0	294	305	2	8	5	318	-317	-7	9	2	805	-894
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7	7	0	321	322	-9	7	5	305	-305	-12	8	1	343	-344	4	8	5	135	-136	-5	9	2	203	198
8	7	0	451	446	-8	7	5	462	-455	-11	8	1	185	-167	5	8	5	149	-165	-4	9	2	249	-253
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10	7	0	-55	8	-6	7	5	104	-112	-9	8	1	143	-138	7	8	5	416	-419	-2	9	2	471	-466
11	7	0	163	158	-5	7	5	332	-323	-8	8	1	128	-114	-12	8	6	311	-306	-1	9	2	837	-836
12	7	0	387	391	-4	7	5	595	-598	-7	8	1	368	-381	-11	8	6	278	-276	0	9	2	465	-468
-12	7	1	158	-164	-3	7	5	600	-598	-6	8	1	711	-714	-10	8	6	143	-135	1	9	2	764	-773

Table 3. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
2	9	2	519	-514	-6	9	8	592	595	7	10	4	205	201	-3	11	3	369	365	-3	12	3	469	476
3	9	2	95	-108	-5	9	8	312	305	-10	10	5	421	-413	-2	11	3	100	101	-2	12	3	471	467
4	9	2	-50	-33	-4	9	8	85	87	-9	10	5	215	-212	-1	11	3	261	256	-1	12	3	242	251
5	9	2	581	-581	-3	9	8	330	334	-8	10	5	136	-126	0	11	3	478	480	0	12	3	308	319
6	9	2	566	-559	-2	9	8	332	338	-7	10	5	235	-230	1	11	3	363	358	1	12	3	189	189
7	9	2	184	-189	-1	9	8	149	146	-6	10	5	335	-325	2	11	3	135	-135	2	12	3	150	158
8	9	2	323	-336	0	9	8	266	266	-5	10	5	133	-123	3	11	3	232	231	3	12	3	421	419
9	9	2	243	-245	1	9	8	440	433	-4	10	5	400	-396	4	11	3	599	621	4	12	3	346	347
-11	9	3	292	285	2	9	8	352	358	-3	10	5	514	-506	5	11	3	-57	41	5	12	3	350	351
-10	9	3	426	436	-7	9	9	200	-194	-2	10	5	366	-355	6	11	3	81	68	-8	12	4	-59	42
-9	9	3	128	130	-6	9	9	265	-259	-1	10	5	232	-235	7	11	3	278	289	-7	12	4	226	219
-8	9	3	254	260	-5	9	9	162	-171	0	10	5	-69	-2	-9	11	4	162	169	-6	12	4	-59	64
-7	9	3	344	344	-4	9	9	280	-276	1	10	5	136	-140	-8	11	4	462	461	-5	12	4	80	-80
-6	9	3	176	179	-3	9	9	264	-256	2	10	5	418	-415	-7	11	4	141	141	-4	12	4	217	225
-5	9	3	565	564	-2	9	9	307	-305	3	10	5	237	-249	-6	11	4	110	111	-3	12	4	265	260
-4	9	3	177	151	-1	9	9	174	-183	4	10	5	209	-210	-5	11	4	212	207	-2	12	4	92	-90
-3	9	3	396	402	0	10	0	560	554	5	10	5	385	-392	-4	11	4	167	173	-1	12	4	74	59
-2	9	3	674	667	1	10	0	262	260	-10	10	6	-57	44	-3	11	4	362	359	0	12	4	174	184
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0	9	3	175	170	3	10	0	161	161	-8	10	6	328	-335	-1	11	4	294	290	2	12	4	158	150
1	9	3	370	368	4	10	0	436	440	-7	10	6	144	-144	0	11	4	349	355	3	12	4	-57	-36
2	9	3	332	335	5	10	0	-69	-29	-6	10	6	-53	16	1	11	4	275	274	4	12	4	111	126
3	9	3	609	613	6	10	0	-51	10	-5	10	6	112	-115	2	11	4	-55	54	-7	12	5	353	-334
4	9	3	309	310	7	10	0	79	83	-4	10	6	362	-353	3	11	4	89	88	-6	12	5	302	-311
5	9	3	314	310	8	10	0	398	411	-3	10	6	170	-173	4	11	4	258	255	-5	12	5	211	-211
6	9	3	383	389	9	10	0	249	238	-2	10	6	179	179	5	11	4	287	289	-4	12	5	202	-192
7	9	3	99	108	10	10	0	82	-76	-1	10	6	299	-303	-9	11	5	96	-90	-3	12	5	118	-126
8	9	3	86	87	-10	10	1	454	-441	0	10	6	271	-266	-8	11	5	234	-239	-2	12	5	423	-426
9	9	3	165	166	-9	10	1	383	-381	1	10	6	121	-113	-7	11	5	336	-347	-1	12	5	453	-459
-11	9	4	-55	28	-8	10	1	259	-258	2	10	6	-54	-8	-6	11	5	272	-270	0	12	5	306	-309
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-4	9	4	554	554	-1	10	1	627	-628	-5	10	7	315	326	1	11	5	391	-397	-2	12	6	160	-167
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1	9	4	-51	4	4	10	1	220	-218	0	10	7	267	269	-7	11	6	300	-307	2	13	0	201	203
2	9	4	771	784	5	10	1	384	-389	1	10	7	239	243	-6	11	6	216	-215	3	13	0	141	149
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5	9	4	178	175	8	10	1	195	-191	-6	10	8	117	117	-3	11	6	135	-141	6	13	0	-57	17
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4	9	5	246	-249	7	10	2	120	-114	-7	11	1	170	-160	5	12	0	159	159	0	13	2	245	-254
5	9	5	-55	12	8	10	2	-53	-4	-6	11	1	394	-397	6	12	0	158	155	1	13	2	209	-220
6	9	5	425	-429	-11	10	3	118	96	-5	11	1	561	-570	7	12	0	68	65	2	13	2	145	-148
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-6	9	6	70	-72	-4	10	3	586	599	2	11	1	398	-404	-2	12	1	94	-94	-2	13	3	137	142
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-3	9	6	554	-553	-1	10	3	359	356	5	11	1	64	-53	1	12	1	386	-386	1	13	3	221	224
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1	9	6	240	-249	3	10	3	331	326	-9	11	2	189	-180	5	12	1	94	-87	-4	13	4	155	157
2	9	6	-53	19	4	10	3	213	212	-8	11	2	-55	5	6	12	1	285	-303	-3	13	4	161	161
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5	9	6	472	-477	7	10	3	175	171	-5	11	2	550	-551	-7	12	2	-55	21	0	13	4	88	87
-10	9	7	116	121	8	10	3	469	460	-4	11	2	458	-463	-6	12	2	167	-167	1	13	4	252	269
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-8	9	7	358	353	-9	10	4	366	369	-2	11	2	429	-426	-4	12	2	173	-180	-2	13	5	164	-163
-7	9	7	255	259	-8	10	4	57	-37	-1	11	2	157	-162	-3	12	2	57	2	0	14	0	177	166
-6	9	7	287	287	-7	10	4	-54	-55	0	11	2	89	-76	-2	12	2	71	77	1	14	0	-57	23
-5	9	7	234	227	-6	10	4	292	305	1	11	2	352	-350	-1	12	2	344	-350	2	14	0	85	90
-4	9	7	159	166	-5	10	4	300	288	2	11	2	214	-210	0	12	2	146	-142	3	14	0	146	136
-3	9	7	573	558	-4	10	4	96	105	3	11	2	489	-484	1	12	2	113	120	-3	14	1	230	-234
-2	9	7	109	111	-3	10	4	131	-137	4	11	2	470	-459	2	12	2	162	-164	-2	14	1	502	-515
-1	9	7	74	78	-2	10	4	395	401	5	11	2	-54	-21	3	12	2	266	-278	-1	14	1	472	-465
0	9	7	464	457	-1	10	4	347	344	6	11	2	166	-165	4	12	2	-55	20	0	14	1	230	-234
1	9	7	269	270	0	10	4	-52	-4	7	11	2	136	-140	5	12	2	114	-90	1	14	1	178	-181
2	9	7	191	183	1	10	4	84	80	-9	11	3	159	157	6	12	2	72	-74	2	14	1	186	-183
3	9	7	253	244	2	10	4	290	289	-8	11	3	526	541	-8	12	3	288	285	-3	14	2	-54	4
4	9	7	154	153	3	10	4	329	325	-7	11	3	-57	31	-7	12	3	295	305	-2	14	2	78	50
-9	9	8	-57	30	4	10	4	-54	34	-6	11	3	-54	18	-6	12	3	-58	41	-1	14	2	84	-82
-8	9	8	270	272	5	10	4	84	-80	-5	11	3	382	382	-5	12	3	290	274	0	14	2	123	-122
-7	9	8	267	266	6	10	4	197	187	-4	11	3	448	451	-4	12	3	384	386	1	14	2	-56	-14

RESULTS

Fig. 1. is a stereoscopic view of the hexathionate ion as seen along an approximate twofold axis, and Fig. 2 is a view normal to this axis, with principal bond lengths and angles as calculated from the atomic coordinates of Table 1.

Fig. 1. The *cis-cis* form of the hexathionate ion in $K_2Ba(S_6O_6)_2$ as seen along an approximate twofold axis. The ellipsoids represent 50 % probability.

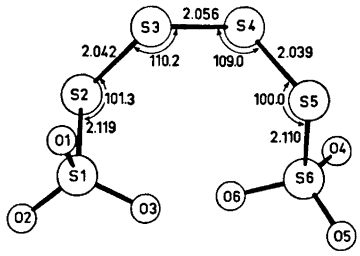

Fig. 2. The hexathionate ion as seen normal to an approximate twofold axis.

The differences between the dimensions of the hexathionate ion listed in Table 4, and those arrived at by the refinement based on two-dimensional film data,[1] are within the errors estimated for the latter. The standard deviations given in parentheses in Table 4 are about one tenth of those estimated for the film data.

The terminal S – S bonds, 2.119 and 2.110 Å, are between sulphonate sulphur atoms and divalent sulphur atoms, and are considerably longer than the three middle S – S bonds, 2.041, 2.056 and 2.039 Å, which are all between two divalent sulphur atoms. Of these three middle bonds the central one is 0.015 – 0.017 Å longer than the two others.

The dimensions of the hexathionate ion in the *cis-cis* form in the present salt will be further discussed in the next paper[3] and there compared to those of the hexathionate ion in the *trans-trans* form.

The packing in the crystal has been described in detail earlier,[1] and only a few aspects will be repeated here in order to present the redetermined dimensions.

Each barium ion, situated on a twofold axis, has ten oxygen neighbours within 2.960 Å. Eight of these are in a distorted square antiprism arrangement with Ba-O distances of 2.704(2) – 2.894(2) Å. The O – O edges of the square faces are in the range 3.243(3) – 4.117(3) Å, and the O – O edges between the square faces are in the range 3.007(2) – 3.455(3) Å. The O – O – O angles of

Table 4. Dimensions of the *cis-cis* form of the hexathionate ion. Standard deviations, given in parentheses, include estimated uncertainties in unit cell dimensions.

Bond lengths and angles

S(1)–S(2) = 2.1186(11) Å	∠S(1)–S(2)–S(3) = 101.25(5)°
S(2)–S(3) = 2.0415(14)	∠S(2)–S(3)–S(4) = 110.20(5)°
S(3)–S(4) = 2.0561(13)	∠S(3)–S(4)–S(5) = 108.99(5)°
S(4)–S(5) = 2.0394(16)	∠S(4)–S(5)–S(6) = 99.95(5)°
S(5)–S(6) = 2.1098(11)	
S(1)–O(1) = 1.443(2) Å	S(6)–O(4) = 1.435(2) Å
S(1)–O(2) = 1.441(2)	S(6)–O(5) = 1.459(2)
S(1)–O(3) = 1.448(3)	S(6)–O(6) = 1.449(2)
∠S(2)–S(1)–O(1) = 105.1(1)°	∠S(5)–S(6)–O(4) = 107.3(1)°
∠S(2)–S(1)–O(2) = 100.7(1)°	∠S(5)–S(6)–O(5) = 100.6(1)°
∠S(2)–S(1)–O(3) = 107.4(1)°	∠S(5)–S(6)–O(6) = 107.5(1)°
∠O(1)–S(1)–O(2) = 115.5(2)°	∠O(4)–S(6)–O(5) = 115.8(2)°
∠O(1)–S(1)–O(3) = 111.6(2)°	∠O(4)–S(6)–O(6) = 112.8(2)°
∠O(2)–S(1)–O(3) = 115.0(2)°	∠O(5)–S(6)–O(6) = 111.6(2)°

Dihedral angles

S(1)S(2)S(3)/S(2)S(3)S(4) = 109.4°	S(3)S(4)S(5)/S(4)S(5)S(6) = 106.3°
S(2)S(3)S(4)/S(3)S(4)S(5) = 89.0°	
S(3)S(2)S(1)/S(2)S(1)O(1) = 52.6°	S(4)S(5)S(6)/S(5)S(6)O(4) = 66.5°
S(3)S(2)S(1)/S(2)S(1)O(2) = 173.0°	S(4)S(5)S(6)/S(5)S(6)O(5) = 172.0°
S(3)S(2)S(1)/S(2)S(1)O(3) = 66.4°	S(4)S(5)S(6)/S(5)S(6)O(6) = 55.1°
S(2)S(1)O(1)/S(2)S(1)O(2) = 120.4°	S(5)S(6)O(4)/S(5)S(6)O(5) = 121.5°
S(2)S(1)O(1)/S(2)S(1)O(3) = 119.0°	S(5)S(6)O(4)/S(5)S(6)O(6) = 121.6°
S(2)S(1)O(2)/S(2)S(1)O(3) = 120.6°	S(5)S(6)O(5)/S(5)S(6)O(6) = 116.9°

Non-bonded distances

S(1)–S(4) = 4.5525(11)Å	S(2)–S(5) = 4.3872(16)Å	S(3)–S(6) = 4.4505(13) Å
S(1)–S(5) = 4.7099(13)	S(1)–S(6) = 4.8895(11)	S(2)–S(6) = 4.6100(14)

the faces are 78.05(6)°, 87.51(7)°, 94.53(8)°, and 98.52(7)°. The two oxygen atoms not involved in the antiprism arrangement are at 2.960(2) Å from barium, and lie outside the square faces with distances to the corners in the range 2.406(3) – 3.338(2) Å. Fig. 3 is a stereoscopic view of the Ba – O coordination.

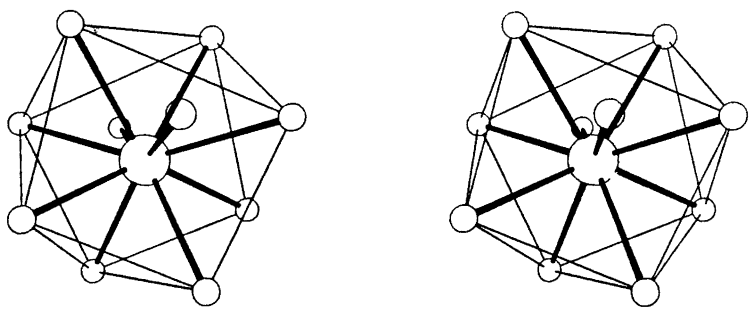

Fig. 3. A stereoscopic view where the barium-oxygen coordination is indicated by the thick lines, and the thin lines are between the oxygen atoms of the square antiprism.

Each potassium ion is surrounded by six oxygen atoms in much distorted octahedral arrangements. The distances from K(1), situated in a symmetry centre, to the oxygen atoms are 2.664(2), 2.781(2), and 3.008(3) Å. The *trans* O – K(1) – O angles are 180.0° and the *cis* O – K(1) – O angles are in the range 48.8(1)° – 131.2(1)°. The distances from K(2), situated on a twofold axis, to the oxygen atoms are 2.668(2), 2.840(2), and 3.028(3) Å. The *trans* O – K(2) – O angles are in the range 132.6(1)° – 159.0(1)° and the *cis* O – K(2) – O angles are in the range 48.0(1)° – 125.6(1)°.

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