

The Crystal Structure of Potassium Triiodidomercurate(II) Monohydrate, $\text{KHgI}_3\text{H}_2\text{O}$

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The crystal structure of $\text{KHgI}_3\text{H}_2\text{O}$ has been determined by single crystal X-ray methods, using three-dimensional diffractometer data. The unit cell is orthorhombic, with $a = 8.625$, $b = 9.345$, and $c = 11.501$ Å. The space group is No. 33: Pna_2_1 . The structure can be described as built up from HgI_4 tetrahedra linked through common corners to infinite chains, running parallel to the a axis of the unit cell. The large differences in the $\text{Hg}-\text{I}$ bond lengths (2.70_5 Å, 2.73_1 Å, 2.83_4 Å, and 2.90_4 Å) indicate deviations from a regular tetrahedral bonding arrangement around the Hg atom.

Mercury(II) can coordinate from one to four halide ions in solution.¹ All evidence points towards a tetrahedral structure for HgX_4^{2-} and a linear arrangement in HgX_2 .²⁻⁴ X-Ray scattering measurements on mercury(II) iodide solutions in dimethylsulfoxide (DMSO) have indicated a pyramidal structure for the HgI_3^- ion and have given no evidence for the formation of polynuclear complexes.⁵ In corresponding mercury bromide solutions, however, polynuclear complexes appear to occur.⁶ Preliminary X-ray scattering measurements on aqueous solutions containing bromide or iodide do not indicate polynuclear complex formation, and even here it seems possible to interpret the results by assuming a pyramidal structure for the HgX_3^- ion.⁷ Other X-ray measurements, however, have been interpreted as indicating the presence of polynuclear complexes in aqueous solutions with less than four iodide ions per mercury ion.⁸

In connection with the X-ray scattering measurements on aqueous solutions of mercury iodide complexes it was of interest to investigate the crystal structure of the compound $\text{KHgI}_3\text{H}_2\text{O}$, which crystallizes from such solutions, since a knowledge of the type of complexes present in the crystal and accurate values for the $\text{Hg}-\text{I}$ bond lengths would be useful in the interpretation of the scattering data.

Crystals of this compound obtained by other authors⁹ have been said to have the composition KHgI_3 ,¹⁰ $\text{KHgI}_3\text{H}_2\text{O}$,^{11,10} or $\text{KHgI}_3(\text{H}_2\text{O})_{1.5}$.¹² According

to Pernot,¹¹ the composition is $\text{KHgI}_3\text{H}_2\text{O}$. She obtained no evidence for the formula KHgI_3 , and attributed the formula $\text{KHgI}_3(\text{H}_2\text{O})_{1.5}$ to insufficiently dry crystals. The formula $\text{KHgI}_3\text{H}_2\text{O}$ is in agreement with the results of the present work.

EXPERIMENTAL

Preparation of crystals. Crystals were prepared by dissolving 9.74 g HgI_2 (Baker analyzed) and 6.26 g KI (E. Merck, Darmstadt, zur Analyse) in 4.0 ml of H_2O at about 60°C, to give a molar ratio of $\text{KI}:\text{HgI}_2 = 1.76$. The iodide content had to be kept high, otherwise a mixture of HgI_2 and $\text{KHgI}_3\text{H}_2\text{O}$ was obtained on cooling. The red mercury(II) iodide dissolved readily, yielding a heavy yellow solution which on cooling deposited yellow crystals of trapezoidal cross-section. The crystals were filtered off and dried over silica gel in a desiccator. They are very soluble in water and ethanol, but insoluble in benzene and carbon tetrachloride. They are decomposed slowly by light, but seem to be fairly stable if kept in a desiccator in the dark.

Analysis. The analysis was carried out according to the method described by Pernot.¹¹ A glass tube drawn out into two bulbs 2 cm apart was weighed empty, the crystals were inserted in the end bulb, and the tube was weighed again. The tube was then held horizontal, and the bulb carefully warmed to drive off the water of crystallization which condensed near the end of the tube. The bulb was then heated more strongly, until mercury(II) iodide sublimed into the second bulb. When the violet colour of liberated iodine was just perceptible in the end bulb, the heating was stopped. The tube was then dried and weighed, the water content being obtained from the loss in weight. The bulbs containing potassium iodide and mercury(II) iodide, respectively, were then separated, and the separate pieces weighed, cleaned and reweighed to obtain the amounts of potassium iodide and mercury(II) iodide present. The results indicated, however, that the separation of KI and HgI_2 by this method was not complete, and the potassium content was therefore determined separately by atomic absorption spectroscopy, using a Perkin Elmer 303. Crystals of known weight were dissolved in a known amount of water. In contact with water, the crystals decomposed and red mercury(II) iodide precipitated. An aliquot was taken from the clear solution and diluted so as to give a potassium content of approximately 4 ppm. Potassium chloride was used as standard, and the range of measurement was 2–6 ppm K.

The density of the crystals was estimated according to the method of Archimedes as described by Schrewelius.¹⁰ The average of six determinations was $4.57 \pm 3 \text{ g/cm}^3$.

The results of the analysis, which are summarized in Table 1, support the conclusion reached by Pernot,¹¹ that the composition of the crystals is $\text{KHgI}_3\text{H}_2\text{O}$.

Table 1. Result of the analysis.

Substance	Observed (%)	Calculated (%) for $\text{KHgI}_3\text{H}_2\text{O}$
H_2O	2.65	2.823
KI + HgI_2	97.15	97.177
K	6.43	6.123
Density	4.57	4.574 ($z=4$)

INTENSITY DATA

The crystals, which are acicular (needle-axis parallel to the crystallographic a axis), were cut to approximately cubic dimensions. The cube edge was, in all cases, approximately 0.1 mm. Single crystals were mounted about the a and b

axes, and the layers $h0l-h6l$ (402 reflections) and $0kl-3kl$ (370 reflections) were recorded, using multiple film equi-inclination Weissenberg techniques and Ni-filtered $\text{Cu}K$ radiation. From a crystal mounted along a face diagonal ([011]) as rotation axis, 246 reflections were similarly recorded from the zero, second and fourth layers.

The relative intensities of the reflections were estimated visually by comparison with a scale prepared by making timed exposures of a selected reflection from the relevant crystal.

Although these data proved to be sufficient for the determination of the main features of the structure, they were not sufficient for an unambiguous location of the oxygen atoms. For the final refinement of the structure, a new set of intensity data was therefore recorded, using an automatic diffractometer (type Philips-Norelco PAILRED) with a scintillation counter and $\text{Mo}K$ radiation, monochromatized with a crystal of lithium fluoride. Half the sphere of reflection was explored ($0kl-10kl$), and a total of 1542 reflections were recorded. The crystal used had the dimensions 0.14 mm in the direction of the a axis, and 0.11 mm in the other two axial directions. The intensity values were corrected for absorption, assuming a linear absorption coefficient of 274 cm^{-1} .

All calculations were carried out on a CDC3600 or an IBM360/50 computer. The following programs were used:

- DATAP2: LP and absorption correction of Weissenberg and diffractometer data.¹³
DRF: Structure factor calculations and Fourier summations.¹⁴
LALS: Full matrix least squares refinement.¹⁵
DISTAN: Calculation of interatomic distances and angles.¹⁶
POWDER: Least squares refinement of unit cell parameters from powder photographs.¹⁷

UNIT CELL AND SPACE GROUP

From the Weissenberg photographs, the Laue symmetry was found to be mmm . Approximate unit cell dimensions were estimated from the rotation and Weissenberg photographs, and more accurate dimensions were obtained from a Guinier powder photograph taken with $\text{Cu}K\alpha$ radiation ($\lambda(\text{Cu}K\alpha_1)=1.54051 \text{ \AA}$), using lead(II) nitrate ($a_0=7.8566 \text{ \AA}$) as an internal standard.¹⁸ A least squares refinement led to the values $a=8.6252 (11)$, $b=9.3445 (11)$, $c=11.5008 (10)$, $V=926.95 \text{ \AA}^3$. Observed and calculated $\sin^2\theta$ values are listed in Table 2.

Assuming four formula units in the unit cell, the calculated density is 4.574 g/cm^3 , which is in agreement with the observed values of 4.57 g/cm^3 (Table 1).

Systematically absent reflections are $0kl$ with $k+l$ odd, and $h0l$ with h odd. This is in accordance with the orthorhombic space groups:¹⁹ No. 33, $Pna2_1$, and No. 62, $Pnam$. All reflections hkl with $k+l$ odd are very weak, which indicates an approximate A-centering of the unit cell, at least with respect to the mercury and the iodine atoms.

Table 2. Powder photograph of $\text{KHgI}_3\text{H}_2\text{O}$. $\text{CuK}\alpha_1$ radiation, $\lambda(\text{CuK}\alpha_1) = 1.54051 \text{ \AA}$. Internal standard lead(II) nitrate ($a_0 = 7.8566 \text{ \AA}$). $a = 8.6252 \text{ \AA}$, $b = 9.3445 \text{ \AA}$, $c = 11.5008 \text{ \AA}$, cell volume = 926.95 \AA^3 .

$h k l$	$10^6 \sin^2 \theta$ calc	$10^6 \sin^2 \theta$ obs	I obs	$h k l$	$10^6 \sin^2 \theta$ calc	$10^6 \sin^2 \theta$ obs	I obs
0 1 1	1129	1125	vs	3 3 2	15086	15086	s
0 0 2	1795	1791	m	2 1 5	15090		
1 1 1	1926	1923	m	0 0 6	16157	16145	w
0 2 0	2717	2714	m	3 2 4	17075	17067	w
2 0 0	3190	3188	m	4 2 2	17272	17261	m
1 2 0	3515	3505	vvw	0 3 5	17334	17341	m
2 1 1	4318	4309	s	3 3 3	17330	17341	m
0 2 2	4512	4505	s	3 4 0	18046		
2 0 2	4985	4978	vvs	0 4 4	18049	18024	w
1 2 2	5310	5304	s	0 2 6	18874	18859	vw
1 1 3	5516	5511	vs	3 1 5	19077	19075	vvw
2 2 0	5907	5894	w	4 3 1	19322		
0 3 1	6562	6557	s	2 0 6	19347	19337	vvw
0 0 4	7181	7177	s	3 4 2	19341	19838	w
1 3 1	7360	7352	w	2 5 1	20620	20633	vvw
2 1 3	7908	7907	s	0 5 3	21021	21024	vvw
3 1 1	8305	8297	m	5 2 0	22654		
1 3 2	8706	8698	vvw	4 2 4	22658	22653	vw
3 2 0	9894	9871	m	0 1 7	22671		
0 2 4	9898			3 5 1	24608		
0 3 3	10153	10138	w	5 1 3	24655	24626	w
2 0 4	10371	10358	w	4 1 5	24659		
1 2 4	10696	10681	vw	0 4 6	27026	27015	vvvv
1 3 3	10950	10945	m	1 4 6	27823	27819	vvw
1 4 0	11666	11662	s	2 6 2	29439	29454	vvw
3 1 3	11896			5 3 3	30089		
0 1 5	11900	11892	s	4 3 5	30093	30084	w
4 0 0	12759	12752	m	4 2 6	31634	31616	vvw
2 2 4	13038	13088	s	3 5 5	35379	35378	vvw
2 3 3	13343	13343	vs	6 3 3	38861	38855	w
3 3 1	13739	13737	vw	2 1 9	40223	40195	vvvv
4 1 1	13887	13871	m				
4 0 2	14555	14552	w				

STRUCTURE DETERMINATION

The positions of the mercury and the iodine atoms were determined from the three-dimensional Patterson function. It was not possible to explain the observed peaks if the unit cell was assumed to have a center of symmetry. For the non-centrosymmetric space group $Pna2_1$, however, an arrangement of the 4 Hg and the 12 I atoms was found, which was consistent with the peaks in the Patterson function. The derived parameters, assuming the z parameter of the Hg atom to be 1/4, were:

$$\begin{aligned} &4 \text{ Hg in } 0.25 \ 0.21 \ 1/4 \\ &4 \text{ I(1) in } 0.50 \ 0.25 \ 0.09 \\ &4 \text{ I(2) in } 0.25 \ 0.42 \ 0.83 \\ &4 \text{ I(3) in } 0.25 \ 0.42 \ 0.42 \end{aligned}$$

Table 3. Peaks in the three-dimensional Patterson function.

Positions			Height	Assignment of vectors		
				Hg-Hg	Hg-I	I-I
0	0	0	100			
0	0.50	0.50	90	2+2		4+2+4+2
0.50	0.02	0	15			2(+2)
0.50	0.50	0.50	24			2+2
0.50	0.35	0	13			2+2
0.50	0.85	0.50	13			2+2
0.50	0.08	0	25	2		
0.50	0.58	0.50	22	1+1		
0	0.28	± 0.08	13		1+1	
0	0.78	± 0.58	12		1+1	
0	0.22	± 0.16	13		1+1	
0	0.72	± 0.66	14		1+1	
0	0.50	± 0.09	13			2
0	0	± 0.59	14			2
0.25	± 0.49	± 0.34	18		1+1	
0.25	± 0.98	± 0.84	17		1+1	
0.25	± 0.17	± 0.29	12			1+1+1+1
0.25	± 0.67	± 0.79	12			1+1+1+1
0.50	0.12	± 0.43	13		1+1	
0.50	0.63	± 0.93	13		1+1	
0.50	0.38	± 0.34	14		1+1	
0.50	0.87	± 0.84	14		1+1	
0.50	± 0.16	± 0.08	7			1+1
0.50	± 0.66	± 0.58	8			1+1

The assignment of vectors in the three-dimensional Patterson function is given in Table 3.

The derived parameter values correspond to a complete A-centering of the unit cell, and do not, therefore, explain the weak reflections hkl with $k+l$ odd. The first least squares refinement was carried out keeping the x parameters fixed, and including an isotropic temperature factor for each atom, which led to an R factor of 0.22 for the 554 observed reflections. The x parameters were then shifted slightly from their values of $1/4$, and the refinement was continued. A number of cycles using different starting values for these shifts finally led to an optimum agreement, corresponding to an R value of 0.169 for all observed reflections. Of these, 123 belonged to reflections with $k+l$ odd, for which the corresponding R factor was 0.203 ($R = \sum ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum |F_{\text{obs}}|$).

A three-dimensional difference map, based on the parameters from the least squares refinement, was used for the location of the light atoms. The position of the potassium atom could be unambiguously determined as corresponding to the highest peak ($13 \text{ el}/\text{\AA}^3$) in the difference map. Several peaks were of a height expected for an oxygen atom, but geometrical reasoning showed that only one of these was plausible. A new least squares refinement with the potassium atom included led to an R factor of 0.156 for all observed reflections, and of 0.159 for those 123 with $k+l$ odd.

REFINEMENT OF THE STRUCTURE

For the final refinement of the structure, the intensity data recorded with the diffractometer were used. The atomic scattering factors were taken from Doyle and Turner,²¹ and were corrected for the real part of the anomalous dispersion according to Cromer.²² Hughes' weighting scheme²³ was used.

The least squares refinement was started with the previously obtained parameters for the Hg and the I atoms. After three cycles, the *R* factor was 0.15 for 1522 observed reflections, and 0.26 for those 392 reflections with *k+l* odd. In a difference map, calculated using the refined parameter values, the two highest peaks occurred at the positions previously assigned to the potassium and the oxygen atoms.

With all atoms included, a new least squares refinement yielded an *R* value of 0.106 for all observed reflections, and 0.187 for those reflections with *k+l* odd. When anisotropic temperature factors for each atom and the imaginary part of the anomalous dispersion correction were included, the *R* factor dropped to 0.089 for all observed reflections, and to 0.159 for the reflections with *k+l* odd. If 32 weak reflections (19 of which had *k+l* odd), which were given zero weight in the refinement, were excluded, the *R* factors were 0.081 and 0.131, respectively. In the final cycle of refinement, all parameter shifts were less than 10 % of the estimated standard deviations.

A three-dimensional electron density map, calculated using the final parameter values, showed peak heights of 350 el/Å³ for the Hg atom, 210–250 el/Å³ for the I atoms, 47 el/Å³ for the K atom, and 17 el/Å³ for the O atom. In the final difference map, all peaks were below 5 el/Å³, with the exception of a peak close to the mercury position which was 8 el/Å³. Observed and calculated *F* values are compared in Table 7.

DISCUSSION OF THE STRUCTURE

The final parameter values are given in Table 4, and interatomic distances and angles in Table 5. Projections of the structure along the three axes of the unit cell are shown in Fig. 1.

Table 4. Final atomic fractional coordinates and thermal parameters. Space group No. 33, *Pna2₁*.^a Standard deviations within brackets. The temperature factor was calculated as
 $\exp[2\pi^2(-h^2a^{*2}U_{11}-k^2b^{*2}U_{22}-l^2c^{*2}U_{33}-hka^*b^*U_{12}-hla^*c^*U_{13}-klb^*c^*U_{23})]$

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
z	0.2559 (3)	0.2032 (2)	$\frac{1}{2}$	0.044 (1)	0.043 (1)	0.045 (1)	-0.009 (2)	0.023 (2)	-0.008 (2)
I	0.4964 (4)	0.2686 (3)	0.0908 (3)	0.026 (1)	0.039 (1)	0.031 (1)	-0.003 (2)	-0.010 (3)	-0.012 (3)
I	0.2442 (6)	0.4266 (3)	0.8193 (3)	0.052 (2)	0.048 (1)	0.043 (1)	-0.002 (4)	-0.012 (4)	-0.027 (2)
I	0.2400 (6)	0.4214 (3)	0.4075 (3)	0.057 (2)	0.055 (2)	0.043 (1)	0.015 (4)	0.027 (5)	0.028 (3)
	0.0607 (15)	0.1552 (13)	0.6173 (19)	0.049 (6)	0.055 (6)	0.121 (14)	-0.018 (10)	0.006 (18)	-0.013 (17)
	0.3655 (37)	0.1002 (34)	0.6126 (53)	0.040 (17)	0.057 (20)	0.127 (42)	0.051 (30)	-0.103 (56)	0.012 (54)

^a The atomic positions are 4(a) (*x,y,z*), ($\bar{x},\bar{y},\frac{1}{2}+z$), ($\frac{1}{2}-x,\frac{1}{2}+y,\frac{1}{2}+z$), ($\frac{1}{2}+x,\frac{1}{2}-y,z$).

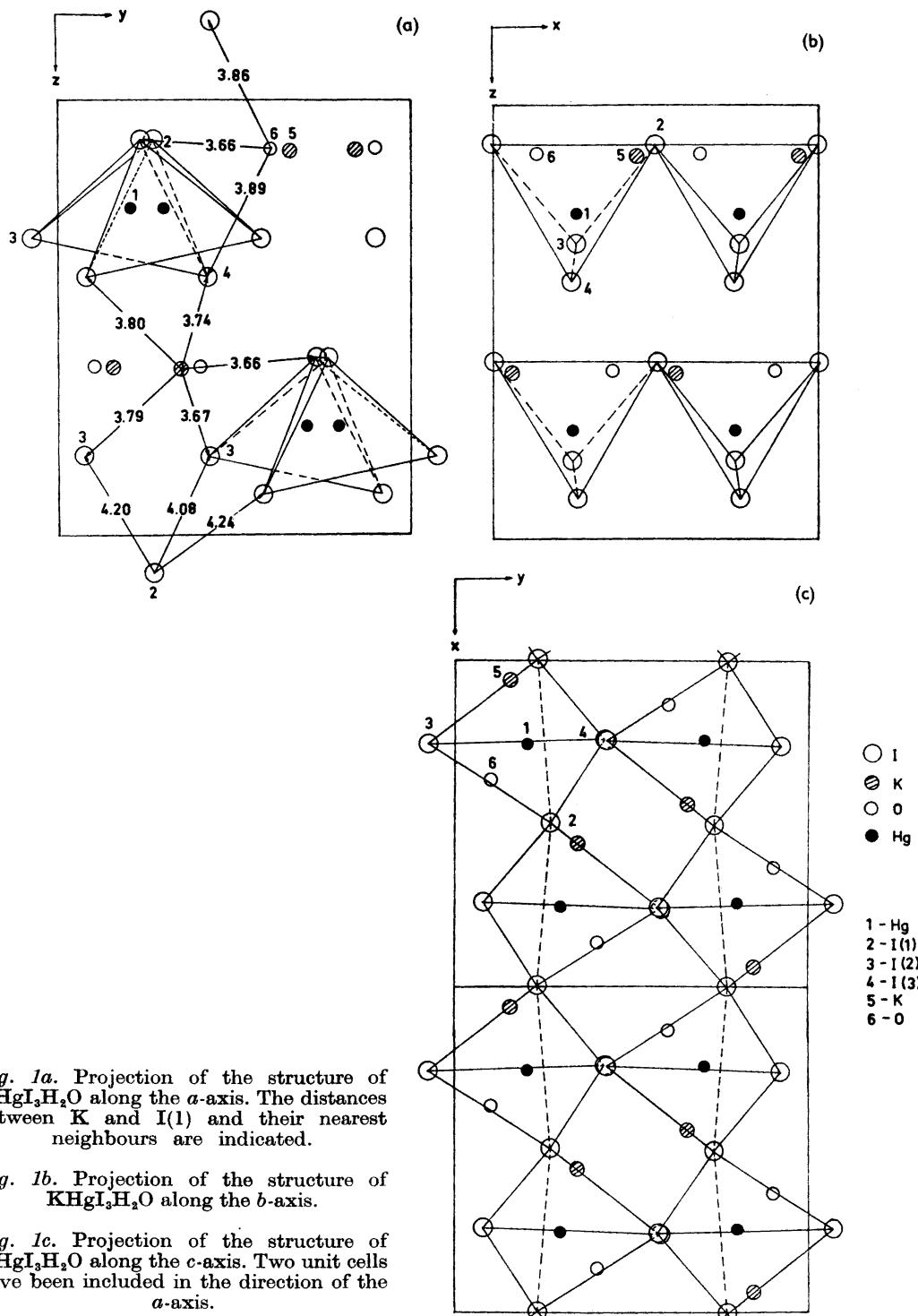


Fig. 1a. Projection of the structure of $\text{KHgI}_3\text{H}_2\text{O}$ along the a -axis. The distances between K and I(1) and their nearest neighbours are indicated.

Fig. 1b. Projection of the structure of $\text{KHgI}_3\text{H}_2\text{O}$ along the b -axis.

Fig. 1c. Projection of the structure of $\text{KHgI}_3\text{H}_2\text{O}$ along the c -axis. Two unit cells have been included in the direction of the a -axis.

Each mercury atom is tetrahedrally coordinated by four iodine atoms, the coordination polyhedron being somewhat distorted (Fig. 2). The tetrahedra are linked through common corners to form chains running parallel to the a axis, as shown in Fig. 1. The Hg—I bond lengths vary between 2.70₅ and 2.90₄ Å, with an average value of 2.79 Å, the two bonds involving the bridging iodine (I(1)) atoms being significantly longer than the other two (Fig. 3).

Table 5a. Atomic distances in $\text{KHgI}_3\text{H}_2\text{O}$. Standard deviations within brackets.

Mercury-iodine distances within the tetrahedron		Iodine-iodine distances within the tetrahedron	
Hg—I(2)	2.705 (3)	I(1)—I(1)	4.326 (1)
—I(3)	2.731 (4)	—I(2)	4.475 (5)
—I(1)	2.834 (4)	—I(2)	4.629 (5)
—I(1)	2.904 (4)	—I(3)	4.494 (5)
		—I(3)	4.564 (5)
		I(2)—I(3)	4.735 (4)
Iodine-iodine distances between different chains		Distances between potassium and its nearest neighbours	
I(1)—I(2)	4.082 (5)	K—O	2.68 (4)
—I(2)	4.200 (5)	—O	2.84 (3)
—I(3)	4.244 (5)	—I(1)	3.66 (1)
—I(3)	4.373 (5)	—I(2)	3.67 (2)
I(2)—I(3)	4.526 (7)	—I(2)	3.79 (2)
—I(3)	4.737 (5)	—I(3)	3.74 (2)
		—I(3)	3.80 (2)
Distances between oxygen and its nearest neighbours			
O—K	2.68 (4)		
—K	2.84 (3)		
—I(1)	3.66 (3)		
—I(2)	3.86 (6)		
—I(3)	3.89 (6)		

Table 5b. Angles around the Hg atom in an HgI_4 tetrahedron. Standard deviations within brackets.

I(1)—Hg—I(1)	97.9 (1)
I(1)—Hg—I(2)	105.8 (1)
I(1)—Hg—I(3)	108.2 (1)
I(1)—Hg—I(2)	113.4 (1)
I(1)—Hg—I(3)	107.7 (1)
I(2)—Hg—I(3)	121.2 (1)

The potassium ions are each surrounded by two water molecules at 2.68 and 2.84 Å, and five iodine atoms from three different chains of HgI_4 tetrahedra at 3.65–3.80 Å. The water molecules are not coordinated to the mercury atoms, but are in contact with potassium ions and iodine atoms at the distances given in Table 5.

Although the crystals of $\text{KHgI}_3\text{H}_2\text{O}$ are formed from solutions in which, presumably, HgI_3^- or $\text{HgI}_3\text{H}_2\text{O}^-$ complexes occur, they do not contain these units, but are built up from infinite complexes in which the mercury atoms are coordinated only to iodine atoms. This is analogous to what has been found in the newly determined structure of $\text{KHgBr}_3\text{H}_2\text{O}$, which is built up from infinite chains of HgBr_4 tetrahedra.²⁴

Table 6. Interatomic distances found in mercury-iodide compounds.

Compound	Hg—I bond (Å)	I—I distances (Å) within a coordination polyhedron	Shortest distance between I atoms belonging to different coordination polyhedra	Reference
HgI_2 (yellow)	2 atoms 2.62 4 » 3.51	4.36–5.24	4.02	25
HgI_2 (red)	4 » 2.783	4.36–4.64	4.14	26
$\beta\text{-Ag}_2\text{HgI}_4$	4 » 2.77	4.47–4.56	4.29	27
$\beta\text{-Cu}_2\text{HgI}_4$	4 » 2.80	4.58–4.65	3.96	27
$(\text{CH}_3)_3\text{SHgI}_3$	3 » 2.69–2.72 2 » 3.52, 3.69	4.53–4.75	4.33	25
$[(\text{CH}_3)_3\text{S}]_2\text{HgI}_4$	4 » 2.68–2.80	4.38–4.52	4.72	28
$\text{KHgI}_3\text{H}_2\text{O}$	4 » 2.71–2.90	4.33–4.74	4.08	Present work

The bonding arrangement around the Hg atom in $\text{KHgI}_3\text{H}_2\text{O}$ is not, however, regularly tetrahedral. The Hg atom is closer to one of the sides of the HgI_4 tetrahedron than to the others. This results in one Hg—I bond being much longer (2.90 Å) than the other bonds (average value 2.75, Å). The I—Hg—I angles in the resulting HgI_3 pyramid (113° , 108° , and 121°) are larger than the other angles around the Hg atom, as shown in Table 5b. This seems to be an indication of a tendency towards a lower coordination of the mercury atom than the tetrahedral one. Discrete HgI_3^- complexes have been found in other structures. In $(\text{CH}_3)_3\text{SHgI}_3$, the HgI_3^- complexes are approximately planar²⁵ with Hg—I bond lengths of 2.69–2.72 Å. The coordination polyhedron of the mercury atom is, however, completed by two more iodine atoms at the much larger distances of 3.52 and 3.69 Å, and is thus a trigonal bipyramidal. Interatomic distances found in a number of mercury iodide compounds are compared in Table 6 with those found in the present structure de-

Table 7. Observed and calculated structure factors. The column headings are the index k , $|F_o|$, $|F_c|$, and α .

0	K	0	5	55	48	321	2	-	18	55	-	19	30	12	-	3	255											
-	1044	356	7	62	69	193	3	160	156	356	10	-	30	119	13	-	19	149										
2	203	219	172	9	56	58	14	4	29	24	275	11	-	15	209	14	-	1	332									
4	49	76	33	11	39	42	135	5	161	161	110	12	-	12	144	15	-	3	43									
6	212	297	177	13	-	15	359	6	69	67	110	13	33	14	195	-	-	-	-									
8	118	122	172	-	-	-	153	151	361	14	-	18	182	-	1	K	13	2	K	2								
10	-	46	344	0	K	0	8	67	73	299	-	1	32	29	110	0	483	590	47	-	-							
12	-	6	71	0	70	80	51	9	39	27	153	1	K	7	-	12	131	1	23	29	175							
14	-	29	350	2	98	94	46	10	36	42	129	1	140	133	199	3	38	36	337	2	250	238	176					
0	K	.1	6	82	94	193	12	33	22	303	0	141	133	173	5	48	50	198	4	125	119	4						
1	331	324	161	8	41	48	296	13	-	12	354	4	35	34	131	6	-	19	156	5	39	33	78					
3	367	393	321	10	33	31	146	14	-	14	117	5	200	197	360	7	41	31	116	6	193	179	259					
5	112	111	119	12	43	30	0	15	-	18	161	6	37	43	318	8	-	12	136	14	-	21	245					
7	42	37	224	-	-	-	7	-	32	33	62	-	1	K	14	-	8	77	73	198	-	-						
9	55	57	27	0	K	11	1	K	2	8	62	-	1	K	14	0	-	14	301	-	-	-	-					
11	55	62	171	1	98	99	28	1	55	52	77	8	54	51	4	66	196	10	58	54	325	-	-					
13	-	20	333	3	73	72	21	2	26	23	290	10	33	31	143	5	-	17	149	11	4	157	-	-				
15	-	3	188	5	41	42	109	3	97	92	248	11	-	8	171	6	-	16	310	2	49	40	124					
0	K	2	7	-	18	242	4	295	290	216	12	-	19	132	7	-	20	277	13	-	2	76	-	-				
2	265	251	145	11	-	26	325	6	152	141	335	14	-	11	310	9	-	14	190	15	-	18	33	-	-			
3	300	374	286	-	-	7	43	-	51	237	-	-	17	-	14	2	-	-	-	-	-	-	-	-				
4	163	149	57	0	K	12	8	96	90	134	-	1	K	9	-	2	K	3	-	-	-	-	-	-				
6	105	98	111	0	164	172	341	9	38	37	55	1	1	K	15	0	22	24	191	-	-	-	-	-				
8	161	152	49	2	94	87	215	10	57	56	62	2	165	161	155	1	46	41	340	1	281	281	163					
10	66	67	186	4	54	53	27	11	35	32	243	2	33	37	92	2	-	23	161	3	406	430	11					
12	38	40	322	6	51	52	142	12	33	26	212	4	56	50	26	-	17	44	4	-	7	347	-	-				
14	36	18	201	3	36	39	14	13	24	22	67	5	38	43	23	4	-	6	60	5	84	61	130					
0	K	2	12	-	17	0	24	15	-	10	243	7	76	68	7	-	16	237	6	-	22	39	-	-				
1	82	76	285	0	K	13	1	K	3	9	-	74	77	7	34	-	37	158	7	44	44	142	-	-				
3	180	173	198	0	K	13	1	K	3	9	-	31	257	8	9	-	13	49	8	-	12	10	-	-				
5	219	197	205	1	90	98	169	1	314	312	22	10	-	16	376	9	-	6	314	0	37	33	240					
7	152	144	5	3	63	80	315	2	-	20	124	11	-	21	80	-	-	10	-	15	187	-	-					
9	63	59	132	5	33	36	149	3	188	174	170	12	-	7	156	-	1	K	16	11	60	54	188	-	-			
11	75	73	1	7	-	9	27	4	54	49	359	13	-	14	265	1	-	3	174	12	-	1	6	-	-			
13	35	25	335	9	43	27	229	5	112	107	306	14	-	8	34	2	-	17	157	13	-	22	341	-	-			
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0	K	3	-	-	-	7	194	-	183	198	1	K	9	4	-	-	19	18	15	-	4	60	-	-				
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4	182	172	199	2	40	46	281	1	49	41	198	1	46	45	11	7	-	12	352	0	250	247	152	-	-			
6	145	136	326	6	-	18	313	12	-	20	154	4	81	81	191	-	2	368	371	311	-	-	1	46	-	-		
8	60	50	164	8	37	42	23	13	-	12	92	6	23	30	33	3	1	K	17	3	-	1	27	-	-			
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12	49	44	156	-	-	15	-	15	-	15	0	8	31	22	214	2	-	7	303	5	-	16	156	-	-			
14	-	3	55	0	K	15	-	-	9	-	-	-	25	215	3	-	14	336	6	68	67	238	-	-	-	-		
0	K	5	-	1	45	2	238	1	K	4	10	-	25	23	4	-	7	128	7	-	17	335	-	-	-	-		
1	320	315	172	5	39	31	195	2	209	185	168	12	-	16	199	6	-	16	296	0	-	6	292	-	-			
3	341	321	77	7	-	31	158	3	81	76	379	13	-	14	31	7	-	21	24	10	51	48	172	-	-			
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7	40	34	305	6	-	15	-	15	-	11	253	7	31	32	145	2	2	K	9	1	304	298	306	-	-			
9	119	112	305	0	K	16	6	177	171	163	1	-	11	310	1	-	1	K	16	13	33	2	324	-	-	-	-	
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2	286	270	0	0	K	17	13	36	19	126	8	63	60	191	0	-	407	174	2	-	19	215	-	-	-	-		
4	131	121	165	1	-	11	212	14	-	17	341	9	-	25	326	1	-	10	188	3	101	67	271	-	-	-	-	
6	40	39	149	3	39	41	238	15	33	10	301	16	36	32	2	151	155	184	4	-	12	337	-	-	-	-		
8	-	18	317	5	-	8	357	11	-	17	149	7	28	23	175	5	-	33	195	3	199	199	278	-	-	-	-	
10	44	47	177	7	41	10	315	1	K	5	12	-	5	373	4	101	101	170	6	-	8	337	-	-	-	-		
12	-	21	172	4	406	451	355	11	36	24	271	8	-	24	281	15	-	3	173	0	115	78	319	-	-	-	-	
14	-	5	177	0	K	18	2	28	23	73	-	21	61	9	-	2	225	9	98	102	149	-	-	-	-	-		
0	K	7	2	38	25	15	4	32	20	229	1	40	36	352	8	188	193	353	10	-	6	341	-	-	-	-	-	
1	320	315	343	4	-	10	215	5	236	228	142	2	-	15	190	9	-	4	168	11	45	47	34	-	-	-	-	-
3	123	117	91	-	-	6	57	52	262	3	43	42	25	176	10	87	86	170	12	-	-	5	134	-	-	-	-	-
5	164	164	347	1	K	0	7	104	100	66	4	-	20	278	11	-	10	354	13	-	22	162	-	-	-	-	-	
7	-	24	80	1	-	22	359	8	59	56	85	66	69	346	12	34	14	334	14	-	2	130	-	-	-	-	-	
9	83	90	191	2	98	98	4	9	55	53	140	6	42	25	99	13	-	0	152	-	-	-	-	-	-	-	-	-
11	-	3	326	3	88	90	178	10	31	34	248	7	48	50	161	14	-	25	170	2	6	326	-	-	-	-	-	
13	-	21	172	4	406	451	355	11	36	24	271	8	-	24	281	15	-	3	173	0	115	78	319	-	-	-	-</td	

Table 7. Continued.

2	K	7	2	-	80	227	11	33	32	239	13	-	14	244	3	-	5	320	5	64	67	162		
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1	168	170	205	4	-	6	53	13	-	18	44	-	-	-	-	37	10	139	7	31	32	304		
2	38	30	26	5	34	21	97	14	-	15	356	3	K	9	-	4	K	0	-	12	145			
3	142	129	173	6	-	34	306	3	K	3	2	29	19	162	1	-	27	174	10	-	13	244		
4	-	9	205	8	-	2	235	1	207	194	3	70	75	181	2	147	164	171	11	33	21	211		
5	83	69	227	9	46	28	184	2	-	19	176	4	-	13	241	3	40	33	354	12	-	5	358	
6	-	20	217	10	-	1	350	3	122	117	3	5	67	71	8	4	103	110	353	13	-	15	337	
7	72	61	147	11	-	18	323	4	-	14	321	6	32	22	64	128	6	162	158	177	-	2	275	
8	-	0	335	11	-	23	61	11	-	25	198	13	-	14	215	12	-	5	116	4	110	102	176	
9	99	101	348	2	K	14	6	44	43	193	8	-	28	199	7	34	35	174	-	4	K	6		
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11	-	19	100	1	-	6	180	8	53	54	10	41	23	31	9	-	4	202	1	36	29	57		
12	-	4	43	2	36	18	249	9	43	31	131	11	-	49	10	43	36	2	222	208	359			
13	-	18	335	3	-	7	57	10	-	34	180	12	-	17	195	11	-	6	164	2	17	174		
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2	K	8	6	34	32	238	13	-	10	296	4	3	K	10	14	-	23	350	6	33	37	24		
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1	-	15	3	8	-	31	165	15	-	15	182	2	2	116	116	-	9	-	9	310				
2	168	163	15	9	-	1	31	-	3	-	19	126	4	K	1	-	4	195						
3	-	3	30	10	-	10	288	3	K	4	63	62	280	0	21	25	285	10	32	35	177			
4	94	92	94	92	-	1	34	94	163	5	29	34	290	1	289	278	152	11	-	4	152			
5	-	40	325	2	K	15	2	231	212	346	6	47	57	173	2	26	26	75	12	-	17	327		
6	92	89	120	0	-	10	199	3	46	41	39	7	-	24	151	3	25	246	323	13	36	4	19	
7	-	9	101	1	50	43	22	4	81	78	18	33	49	4	30	17	17	14	-	5	177			
8	-	23	298	2	-	0	61	8	55	50	96	9	31	24	322	5	60	65	114	-	2	275		
9	33	10	184	3	64	69	356	6	131	131	342	10	-	15	51	6	-	15	255	4	K	7		
10	-	24	167	4	-	2	36	7	46	305	11	-	18	137	7	28	31	238	0	40	27	215		
11	-	24	25	5	-	13	240	8	63	61	167	12	-	6	132	8	27	18	243	1	257	253	343	
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13	-	2	270	7	-	12	117	10	-	16	141	-	-	19	-	16	134	3	99	92	95			
14	-	1	26	8	-	4	38	11	-	29	306	3	K	11	11	50	47	173	4	-	21	62		
2	K	9	0	-	10	155	12	-	8	72	1	29	29	169	12	-	6	344	5	119	120	341		
0	26	19	349	2	K	16	14	-	20	136	2	-	17	57	13	-	16	336	6	-	21	28		
1	182	181	12	6	-	47	170	15	-	14	160	3	32	33	353	14	-	6	270	-	-	21	16	
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3	144	146	154	2	35	9	331	3	K	5	6	-	30	87	4	K	2	10	-	9	4			
4	-	5	167	3	-	1	4	1	202	189	97	56	43	343	0	-	188	198	11	-	3	324		
5	87	87	48	4	37	26	163	2	39	46	173	8	-	25	261	1	54	49	311	12	-	8	200	
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7	-	7	183	7	-	9	322	4	67	67	77	10	-	19	90	3	52	57	259	14	-	2	275	
8	37	23	34	R	-	2	5	5	204	196	322	11	36	6	314	4	152	148	92	-	4	199		
9	-	6	255	3	K	0	14	82	6	56	59	245	12	-	12	279	5	6	14	88	4	K	8	
11	39	28	120	2	K	17	8	44	41	238	1	-	3	K	12	7	6	60	116	0	63	60	296	
12	-	2	244	0	-	7	96	9	52	49	321	1	-	19	14	8	117	113	37	2	151	149	131	
13	-	12	205	1	33	39	291	10	41	37	263	2	31	38	87	9	-	15	137	3	29	26	124	
2	K	10	154	299	4	-	4	51	7	18	45	3	94	-	24	240	10	54	51	137	4	106	123	294
0	149	154	299	4	-	17	219	12	-	19	76	4	93	-	94	144	11	10	46	5	-	8	249	
1	25	17	247	5	-	1	276	13	-	20	150	5	-	25	52	12	36	32	329	6	58	63	7	
2	163	168	174	14	-	14	9	249	6	70	354	9	-	29	10	13	-	1	267	7	-	4	199	
3	-	8	255	3	K	0	-	22	176	10	-	8	188	5	55	27	147	-	15	202	8	32	36	217
4	94	97	346	1	93	92	357	3	K	6	8	-	14	227	15	-	3	244	10	10	36	33	20	
5	54	5	315	2	140	149	182	1	30	214	9	-	14	38	-	-	111	112	27	12	44	32	156	
6	76	81	63	3	80	87	176	2	91	80	146	10	38	24	301	4	K	3	11	-	2	233		
7	-	5	174	3	333	357	174	3	61	51	177	11	21	9	111	112	27	12	44	32	156			
8	-	11	62	5	52	48	354	4	68	123	115	351	-	1	89	81	254	13	-	2	103			
9	-	6	41	6	109	107	349	5	44	51	197	3	K	13	2	30	27	147	-	4	199			
10	32	16	357	7	66	77	172	6	109	111	1	35	293	3	134	200	4	K	9	-	37	210		
11	-	2	457	3	39	21	159	7	45	53	172	2	-	15	24	4	43	18	212	0	25	25	138	
12	-	2	29	196	9	46	41	355	8	44	41	33	39	-	32	161	5	142	127	2	1	25	47	
13	-	0	338	10	-	20	354	9	40	37	196	6	-	28	340	6	-	6	227	2	-	25	47	
2	K	11	12	35	30	351	11	-	19	12	6	-	-	-	22	172	8	-	13	196	4	8	232	
9	-	13	213	123	-	19	356	12	-	3	121	7	33	-	29	140	9	41	49	139	5	42	42	
1	94	102	130	14	-	21	167	13	-	13	193	9	-	18	358	10	-	7	319	6	-	9	318	
2	-	7	69	15	-	9	176	-	-	9	-	10	298	11	59	59	1	7	55	55	55	191		
3	76	78	304	-	3	K	7	10	-	14	151	12	-	5	27	8	-	9	343					
4	-	5	231	3	K	1	1	98	94	191	10	-	9	242	13	-	21	155	9	38	46	12		
5	45	40	64	1	184	163	327	2	41	43	35	6	-	14	242	13	-	2	71	10	-	5	202	
6	29	4	129	2	16	16	209	3	131	130	356	4	-	6	236	1	13	12	12	12	-	2	84	
7	-	5	11	68	71	311	5	47	10	172	170	2	-	10	312	6	123	133	78	-	12	157		
8	-	34	11	5	132	137	3	6	41	46	33	39	-	4	113	13	-	24	228	4	4	296		
9	-	3	207	3	75	72	127	7	35	32	244	4	53	59	4	1	121	131	0	51	50	46		
10	-	2	216	7	116	119	165	8	42	40	158	5	-	17	122	2	131	121	199	0	51	50	46	
11	-	30	169	7	116	119	165	8	42	40	158	5	-	17	122	2	131	121	199	0	51	50	46	
12	-	1	5	8	53	50	30	9	53	48	170	6	-</											

Table 7. Continued.

5	37	35	96	6	34	30	264	5	117	121	355	6	K	1	2	49	45	26	6	K	15							
6	-	5	22	6	92	93	187	6	-	33	280	84	K	1	3	67	72	165	-	17	193							
7	-	17	266	6	36	37	103	7	32	19	73	0	119	108	56	5	38	16	205	0	-	32	198					
8	-	9	225	7	47	105	340	8	33	31	107	1	39	33	163	6	-	24	227	2	-	1	357					
9	-	24	141	8	34	41	284	9	49	37	353	2	72	71	209	7	38	43	140	3	45	45	174					
10	-	5	79	9	32	24	157	10	31	3	27	32	4	-	12	72	8	-	0	153	4	4	39					
11	-	21	322	10	-	30	125	11	-	18	142	5	63	58	118	9	54	64	345	5	-	11	226					
12	-	3	221	11	-	11	125	12	-	22	176	6	-	14	45	10	-	4	214	6	-	5	324					
			12	37	21	132	13	-	22	176	7	65	62	916	11	-	13	112	7	-	8	95						
			13	-	11	340	5	-	13	182	12	33	13	182	9	-	13	112	7	-	8	38						
			14	K	12	13	-	15	123	4	61	59	111	9	37	49	54	13	-	12	331	6	K	16				
			15	-	6	242	15	-	13	163	5	23	64	10	-	43	347	-	6	K	8	0	46	34	166			
			16	-	77	212	-	17	21	3	55	58	101	-	43	337	6	K	8	0	46	34	6	61				
			17	-	19	354	5	K	2	4	38	49	197	12	-	5	247	0	84	90	232	1	-	6	36	378		
			18	-	44	27	1	54	48	71	5	65	59	192	13	-	12	152	1	29	28	181	2	40	36	378		
			19	-	9	13	2	164	155	291	6	42	43	214	14	-	1	87	2	101	101	16	-	-	-	-		
			20	-	35	44	142	3	45	47	216	7	52	55	310	-	3	-	5	282	7	K	9	-	-			
			21	-	9	213	4	168	165	207	8	-	27	214	2	4	58	54	205	1	38	41	353	-	-			
			22	-	30	120	5	44	48	71	9	-	22	210	6	K	2	40	5	-	13	320	2	28	33	188		
			23	-	6	86	6	105	95	333	10	-	2	153	1	26	32	160	6	55	57	116	3	33	34	170		
			24	-	9	337	7	68	62	242	11	-	11	212	3	136	131	174	7	-	17	247	5	32	36	322		
			25	-	6	190	8	46	52	148	12	-	9	19	4	81	82	82	9	-	15	14	6	50	51	174		
			26	-	4	13	10	40	58	-	36	38	65	13	-	3	34	74	10	-	14	152	7	8	69	174		
			27	-	5	146	11	-	18	243	-	5	35	34	74	10	-	6	43	8	-	-	19	163	-			
			28	-	71	80	166	12	-	17	35	1	28	21	287	7	20	228	12	-	20	321	9	-	30	355		
			29	-	9	76	13	-	16	77	2	85	84	19	8	41	49	193	13	-	3	251	10	50	40	353		
			30	-	57	65	315	14	-	11	174	3	-	27	180	8	-	18	327	-	-	11	-	-	9	179		
			31	-	5	288	15	-	8	257	4	50	50	103	10	35	31	331	6	K	9	12	-	14	350	-		
			32	-	5	26	146	5	K	3	3	36	38	16	11	-	9	205	0	-	29	342	13	-	10	358		
			33	-	8	233	5	K	3	6	37	50	355	12	-	24	127	1	114	119	11	14	-	10	165	-		
			34	-	7	14	1	174	159	20	7	-	29	142	12	-	1	56	2	-	8	251	-	-	-	-		
			35	-	6	1	1	13	171	8	38	45	89	13	-	11	26	3	88	89	155	7	K	1	-			
			36	-	8	6	20	47	3	114	16	8	34	20	336	14	-	7	162	1	65	61	335	-	-			
			37	-	9	176	4	44	92	14	10	-	18	238	6	K	3	47	54	36	2	47	46	153	-			
			38	-	10	11	175	9	83	73	232	11	-	13	155	0	27	28	192	6	-	10	77	3	80	77	164	
			39	-	5	51	154	12	-	10	82	5	52	51	343	10	-	18	186	7	-	7	290	10	-	23	112	
			40	-	5	113	114	18	39	29	1	-	114	185	7	-	13	243	8	-	13	187	6	72	72	351		
			41	-	5	71	155	8	39	29	1	5	K	11	2	20	223	229	188	9	-	13	197	6	42	41	130	
			42	-	6	8	25	305	1	32	27	346	4	-	9	347	10	-	10	32	7	64	69	161	-			
			43	-	7	42	49	280	10	34	32	191	2	33	15	23	1	43	17	119	8	-	27	316	-			
			44	-	8	14	267	11	-	11	10	3	40	36	169	8	49	24	17	12	43	17	119	8	-			
			45	-	9	32	33	193	12	-	17	3	4	-	14	333	9	31	25	125	13	-	7	290	10	-		
			46	-	10	5	193	13	-	10	82	5	52	51	343	10	-	18	186	7	-	7	290	10	-	23	112	
			47	-	11	153	14	-	10	82	5	52	51	343	10	-	16	113	11	36	32	2	6	K	10	-		
			48	-	12	33	22	5	K	4	7	37	38	19	12	-	1	351	0	100	29	300	13	-	4	209	-	
			49	-	13	33	22	5	K	4	8	19	20	12	-	14	343	1	272	222	12	100	166	17	-	8	195	-
			50	-	14	32	129	2	K	4	9	14	297	14	-	3	3	3	-	15	241	7	K	2	-			
			51	-	15	32	150	1	K	4	10	122	25	8	-	1	351	0	100	29	300	13	-	4	209	-		
			52	-	16	32	152	2	K	4	11	122	25	8	-	1	343	1	272	222	12	100	166	17	-	8	195	-
			53	-	17	33	47	332	11	K	4	12	140	11	-	1	351	0	100	166	17	-	8	195	-			
			54	-	18	33	47	332	12	K	4	13	140	11	-	1	351	0	100	166	17	-	8	195	-			
			55	-	19	33	47	332	13	K	4	14	124	3	54	5	40	29	242	1	93	88	195	-	-			
			56	-	20	33	47	332	14	K	4	15	124	3	54	5	40	29	242	1	93	88	195	-	-			
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			60	-	24	33	47	332	18	K	4	19	124	3	54	5	40	29	242	1	93	88	195	-	-			
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			64	-	28	33	47	332	22	K	4	23	124	3	54	5	40	29	242	1	93	88	195	-	-			
			65	-	29	33	47	332	23	K	4	24	124	3	54	5	40	29	242	1	93	88	195	-	-			
			66	-	30	33	47	332	24	K	4	25	124	3	54	5	40	29	242	1	93	88	195	-	-			
			67	-	31	33	47	332	25	K	4	26	124	3	54	5	40	29	242	1	93	88	195	-	-			
			68	-	32	33	47	332	26	K	4	27	124	3	54	5	40	29	242	1	93	88	195	-	-			
			69	-	33	33	47	332	27	K	4	28	124	3	54	5	40	29	242	1	93	88	195	-	-			
			70	-	34	33	47	332	28	K	4	29	124	3	54	5	40	29	242	1	93	88	195	-	-			
			71	-	35	33	47	332	29	K	4	30	124	3	54	5	40	29	242	1	93	88	195	-	-			
			72	-	36	33	47	332	30	K	4	31	124	3	54	5	40	29	242	1	93	88	195	-	-			
			73	-	37	33	47	332	31	K	4	32	124	3	54	5	40	29	242	1	93	88	195	-	-			

Table 7. Continued.

termination. In DMSO solutions of mercury(II) iodide, the Hg—I bond lengths have been found to be 2.80 Å in the HgI_4^{2-} complex, and 2.73 Å in the HgI_3^- complex.⁵

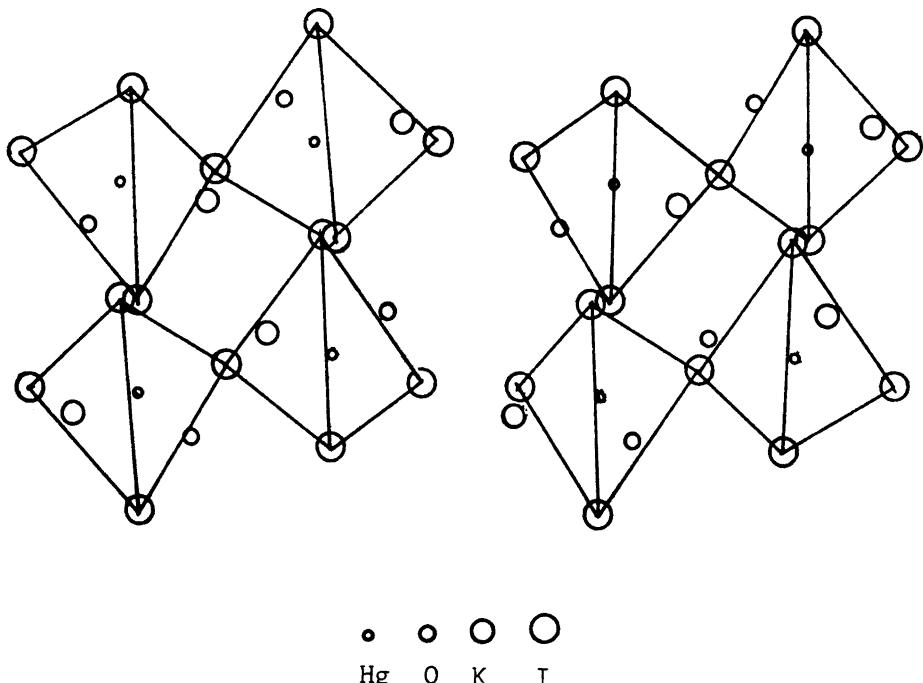


Fig. 2. Stereographic projection of the structure of $\text{KHgI}_3\text{H}_2\text{O}$. The a -axis is parallel to the chain, the b -axis is horizontal, and the c -axis perpendicular.

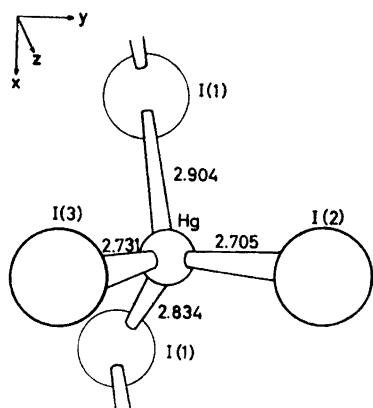


Fig. 3. The configuration of an HgI_4 -group.

Acknowledgements. The authors wish to thank Professor Georg Lundgren for his interest in this work. The work has been supported by the Swedish Natural Science Research Council. Computer time has been made available by the Computer Division of the National Swedish Office for Administrative Rationalization and Economy.

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Received October 1, 1970.