The Crystal Structure of Potassium Triiodidomercurate(II) Monohydrate, KHgI₃H₂O

LARS NYQVIST and GEORG JOHANSSON

Department of Inorganic Chemistry, Chalmers University of Technology and the University of Göteborg, P.O. Box, S-402 20 Göteborg 5, and Department of Inorganic Chemistry, Royal Institute of Technology, S-100 44 Stockholm 70, Sweden

The crystal structure of $KHgI_3H_2O$ 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: $Pna2_1$. 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 $Hg-I$ 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 $KHgI_3H_2O$, which crystallizes from such solutions, since a knowledge of the type of complexes present in the crystal and accurate values for the $Hg-I$ bond lengths would be useful in the interpretation of the scattering data.

Crystals of this compound obtained by other authors [9] have been said to have the composition $KHgI_3$,[10] $KHgI_3H_2O$,[11,10] or $KHgI_3(H_2O)_{1.5}$.[12] According

to Pernot,[11] the composition is $KHgI_3H_2O$. She obtained no evidence for the formula $KHgI_3$, and attributed the formula $KHgI_3(H_2O)_{1.5}$ to insufficiently dry crystals. The formula $KHgI_3H_2O$ 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 $KI:HgI_2 = 1.76$. The iodide content had to be kept high, otherwise a mixture of HgI_2 and $KHgI_3H_2O$ 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.[20] The average of six determinations was 4.57 ± 3 g/cm³.

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 $KHgI_3H_2O$.

Table 1. Result of the analysis.

Substance	Observed (%)	Calculated (%) for $KHgI_3H_2O$
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 CuK 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 MoK 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 $CuK\alpha$ radiation ($\lambda(CuK\alpha_1) = 1.54051$ Å), using lead(II) nitrate ($a_0 = 7.8566$ Å) 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), $V = 926.95$ Å^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 $KHgI_3H_2O$. $CuK\alpha_1$ radiation, $\lambda(CuK\alpha_1) = 1.54051$ Å. Internal standard lead(II) nitrate $(a_0 = 7.8566$ Å). $a = 8.6252$ Å, $b = 9.3445$ Å, $c = 11.5008$ Å, cell volume = 926.95 Å³.

h k l	$10^5\sin^2\theta$ calc	$10^5\sin^2\theta$ obs	I obs	h k l	$10^5\sin^2\theta$ calc	$10^5\sin^2\theta$ 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⎤	18024	w
2 0 2	4985	4978	vvs	0 4 4	18049⎦		
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⎤	19337	vvw
0 3 1	6562	6557	s	2 0 6	19347⎦		
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⎤	22653	vw
1 3 2	8706⎦	8698	vvw	4 2 4	22658⎬		
3 2 0	9894⎤	9871	m	0 1 7	22671⎦		
0 2 4	9898⎦			3 5 1	24608⎤	24626	w
0 3 3	10153	10138	w	5 1 3	24655⎬		
2 0 4	10371	10358	w	4 1 5	24659⎦		
1 2 4	10696	10681	vw	0 4 6	27026	27015	vvvw
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⎤	11892	s	5 3 3	30089⎤	30084	w
0 1 5	11900⎦			4 3 5	30093⎦		
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	vw
3 3 1	13739	13737	vw	2 1 9	40223	40195	vvvw
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:

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

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 $(R = \sum||F_{obs}| - |F_{calc}||/\sum|F_{obs}|)$.

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 el/$Å^3$) 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 scheme [23] 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/Å^3 for the Hg atom, $210-250$ el/Å^3 for the I atoms, 47 el/Å^3 for the K atom, and 17 el/Å^3 for the O atom. In the final difference map, all peaks were below 5 el/Å^3, with the exception of a peak close to the mercury position which was 8 el/Å^3. 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.

ible 4. Final atomic fractional coordinates and thermal parameters. Space group No. 33, $Pna2_1$.[a] Standard deviations within brackets. The temperature factor was calculated as

$$\exp 2\pi^2(-h^2a^{*2}U_{11}-k^2b^{*2}U_{22}-l^2c^{*2}U_{33}-hka^*b^*U_{12}-hla^*c^*U_{13}-klb^*c^*U_{23})$$

om	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
ζ	0.2559 (3)	0.2032 (2)	¼	0.044 (1)	0.043 (1)	0.045 (1)	−0.009 (2)	0.023 (2)	−0.008 (2)
l)	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)
?)	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)
ƚ)	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), $(\bar{x},\bar{y},\tfrac{1}{2}+z)$, $(\tfrac{1}{2}-x,\tfrac{1}{2}+y,\tfrac{1}{2}+z)$, $(\tfrac{1}{2}+x,\tfrac{1}{2}-y,z)$.
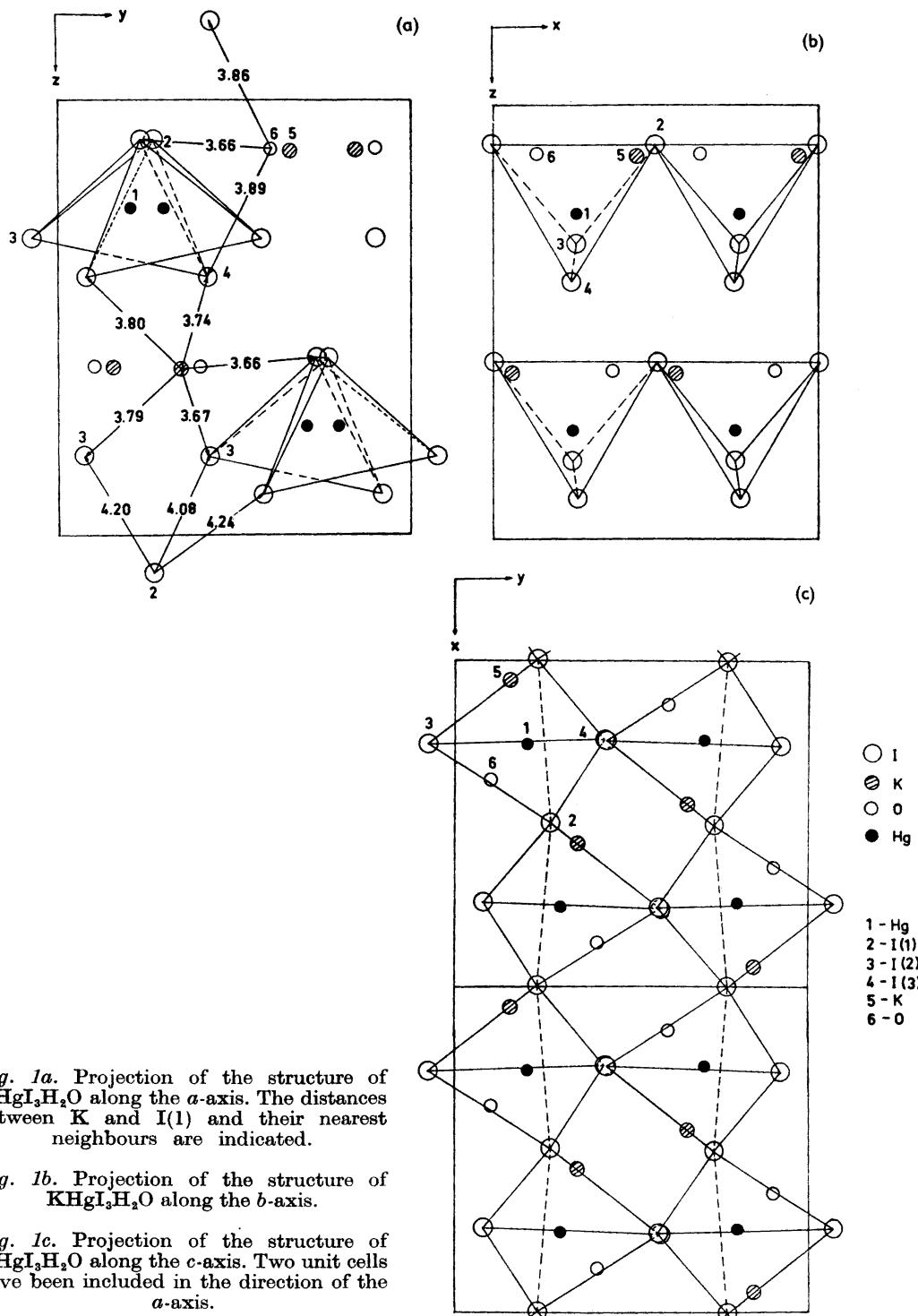
*Fig. 1a.* Projection of the structure of KHgI$_3$H$_2$O along the *a*-axis. The distances between K and I(1) and their nearest neighbours are indicated.

Fig. 1b. Projection of the structure of KHgI$_3$H$_2$O along the *b*-axis.

Fig. 1c. Projection of the structure of KHgI$_3$H$_2$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 2.70_5 and 2.90_4 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 $KHgI_3H_2O$. 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 KHgI$_3$H$_2$O are formed from solutions in which, presumably, HgI$_3^-$ or HgI$_3$H$_2$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 KHgBr$_3$H$_2$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	4.36 – 5.24	4.02	25
	4 »	3.51			
HgI$_2$(red)	4 »	2.783	4.36 – 4.64	4.14	26
β-Ag$_2$HgI$_4$	4 »	2.77	4.47 – 4.56	4.29	27
β-Cu$_2$HgI$_4$	4 »	2.80	4.58 – 4.65	3.96	27
(CH$_3$)$_3$SHgI$_3$	3 »	2.69 – 2.72	4.53 – 4.75	4.33	25
	2 »	3.52, 3.69			
[(CH$_3$)$_3$S]$_2$HgI$_4$	4 »	2.68 – 2.80	4.38 – 4.52	4.72	28
KHgI$_3$H$_2$O	4 »	2.71 – 2.90	4.33 – 4.74	4.08	Present work

The bonding arrangement around the Hg atom in KHgI$_3$H$_2$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$_4$ Å) than the other bonds (average value 2.75$_7$ 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 (CH$_3$)$_3$SHgI$_3$, the HgI$_3^-$ complexes are approximately planar[25] 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 bipyramid. 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.

[Extensive multi-column table of structure factors]

Table 7. Continued.

[Table of structure factor data: columns of h, Fo, Fc, l arranged in blocks labelled by K index. The numerical data is dense and organized in multiple vertical groups across the page.]

Table 7. Continued.

5	37	35	96	4	34	30	264	5	117	121	355				2	49	45	26
6	-	5	22	5	92	93	187	6	-	33	288	0	6 K 1		3	67	72	165
7	-	17	266	6	36	37	103	7	32	19	73	1	84	77	318	4	-	16	205	0
8	-	9	225	7	97	105	340	8	33	31	107	2	119	108	56	5	38	47	230	1
9	-	24	141	8	34	41	284	9	49	37	353	3	39	33	163	6	-	24	227	2
10	-	5	79	9	32	24	159	10	37	27	332	4	72	71	209	7	38	43	140	3

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]

Hg   O   K   I
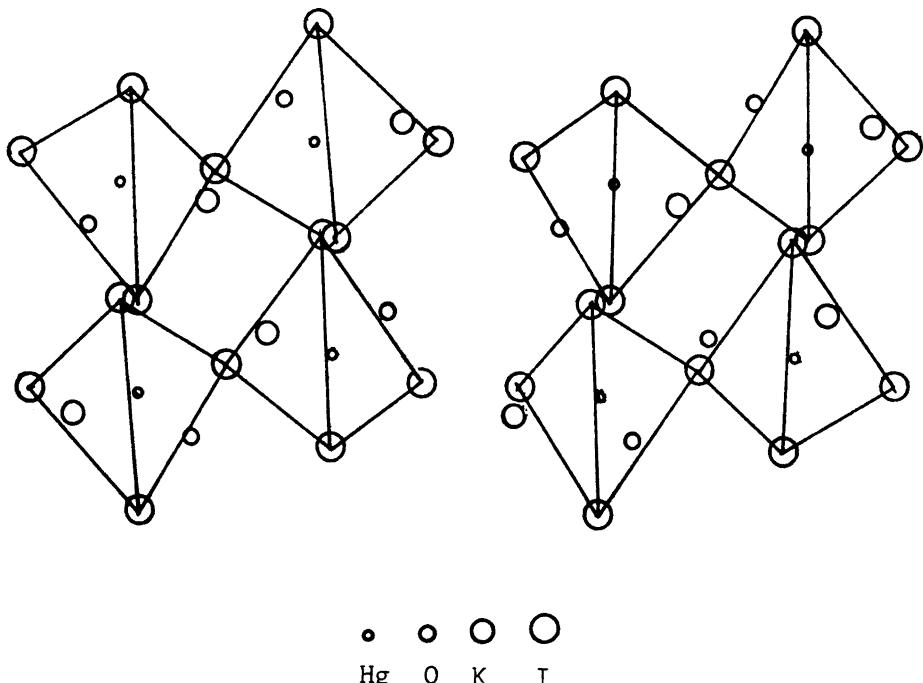
Fig. 2. Stereographic projection of the structure of $KHgI_3H_2O$. The *a*-axis is parallel to the chain, the *b*-axis is horizontal, and the *c*-axis perpendicular.
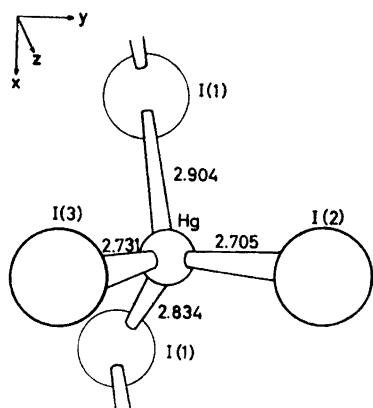
Fig. 3. The configuration of an HgI_4-group.

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