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probably a ${}^1A_{1g}$ as in Fig. 1 in most if not all cases. A study of magnetic properties of various B_2R_6 at various temperatures would help to decide this.

If $2BR_3$ is more stable than B_2R_6 , this means that the lowest B_2R_6 energy is close to or higher than the energy of $2BR_3$. In case the difference is not large, as is probably often true, then, if it is feasible to heat the substance sufficiently, a fraction of the molecules should go over into (one or more of the states of) B_2R_6 . Similarly on heating a substance of the type B_2R_6 , a fraction of the molecules should of course go over into BR_3 . Other fractions should also go into some of the low excited states of B_2R_6 appearing in Fig. 1. Since some of these are paramagnetic, the substance should begin to show paramagnetism if

the temperature can be raised sufficiently without decomposition.

Measurements of magnetic susceptibilities of substances of the B_2R_6 and even perhaps some of those of the BR_3 type (e.g., $B(CH_3)_3$) should give interesting results, especially if temperatures can be raised. Studies leading to determinations of the splitting energies of B_2R_6 into $2BR_3$ would naturally also be of interest. An investigation of the photographic infrared absorption spectrum of B_2H_6 , in order to look for the probably expected ${}^1A_{1g} \rightarrow {}^1E_u$ bands, is being undertaken at this University.

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The Structure of Potassium Hexachlorothalliate Dihydrate

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Potassium hexachlorothalliate dihydrate is shown from x-ray data to possess a body centered tetragonal unit of structure with $a_0 = 15.841 \pm 0.020\text{\AA}$, $c_0 = 18.005 \pm 0.020\text{\AA}$ containing $14 K_3TiCl_6 \cdot 2H_2O$. A structure with nineteen determinable parameters is developed from $D_{4h}^{17} - I 4/mmm$, and accounts satisfactorily for observed intensity data. $TiCl_6^{3-}$ ions occur as well-defined groups. 24 of the $42 K^+$ ions are closely surrounded by 8 Cl^- , 16 K^+ by 7 Cl^- and 2 H_2O , and the remaining 2 K^+ by 6 H_2O ; these $K(H_2O)_6^+$ groups are situated in regions of definitely negative potential. The structure is very compact, but has

quite satisfactory interatomic distances throughout. The evidence from this and from a previous structural determination of $Cs_3Ti_2Cl_9$ shows that thallic thallium tends to form six stable covalent bonds with chlorine with a $Tl-Cl$ separation of about 2.55\AA , in agreement with the covalent radii of Pauling and Huggins. It is shown also that a compound of empirical formula $Rb_3TiBr_6 \cdot (8/7)H_2O$ probably possesses essentially the same type of structure as $K_3TiCl_6 \cdot 2H_2O$; dimensional relations in the bromothalliate permit the alkali ions of $2(b)$ to coordinate eight rather than six molecules of water.

INTRODUCTION

THE coordination and bonding properties of such heavy metal forming elements as thallium and lead, lying in the B subgroups of the periodic system, have as yet been comparatively little studied. With a view toward elucidating the characteristic structural properties of trivalent thallium, we have undertaken x-ray studies of a number of its complex salts. The results of one such investigation, dealing with cesium enneachlorodithalliate, $Cs_3Ti_2Cl_9$, have already been reported;¹ we describe in the present paper the structure of potassium hexachlorothalliate dihydrate, $K_3TiCl_6 \cdot 2H_2O$, and summarize briefly

our present knowledge of the structural properties of thallic thallium.

Good crystals of $K_3TiCl_6 \cdot 2H_2O$, from one to two mm on an edge, were prepared without difficulty according to the directions of Meyer.² In habit and in general appearance the crystals seemed to agree closely with the description of Groth,³ who lists them as tetragonal bipyramidal, $c/a = 0.7913$. Laue and oscillation photographs were used as a source of x-ray data.

DETERMINATION OF THE STRUCTURE

The smallest tetragonal unit of structure is one with $a_0 = 15.841 \pm 0.020\text{\AA}$, $c_0 = 18.005$

² Meyer, *Zeits. f. anorg. allgem. Chemie* **24**, 321 (1900).

³ Groth, *Chemische Kristallographie*, Engelmann, Leipzig, **1**, 424 (1908).

¹ Hoard and Goldstein, *J. Chem. Phys.* **3**, 199 (1935).

$\pm 0.020\text{\AA}$, $c_0/a_0 = 1.137$, to be compared with $\sqrt{2} \cdot 0.7913 = 1.119$. This unit accounts for both the oscillation and the numerous Laue data, and may be confidently accepted as the true one.

All of the x-ray data agree with a body centered lattice; the unit must then contain an even number of molecules. Placing 14 $\text{K}_3\text{TlCl}_6 \cdot 2\text{H}_2\text{O}$ within a unit of this size leads to a calculated density of 2.89 g/cm^3 , whereas the reported density⁴ is 2.859 g/cm^3 , and our experimentally determined value, using the flotation method, is $2.90 \pm 0.10 \text{ g/cm}^3$. We conclude, therefore, that the body centered unit contains fourteen, and a primitive unit contains the rather extraordinary number of seven molecules of $\text{K}_3\text{TlCl}_6 \cdot 2\text{H}_2\text{O}$. This conclusion is supported also by x-ray and density data obtained from the apparently isomorphous compound, $\text{Rb}_3\text{TlBr}_6 \cdot (8/7)\text{H}_2\text{O}$, which we discuss briefly in the last paragraph of this section.

The symmetry indicated by the x-ray data is that of D_4^h . All space groups based upon a body centered lattice with special criteria which could give rise to x-ray data of this symmetry are eliminated by the appearance of "forbidden" reflections.⁵ We assume the holohedral space group, $D_{4h}^{17} - I 4/mmm$, in preference to the remaining possibilities which lack centers of symmetry since (1) the face development of the crystals is in agreement with this view, and (2) an experiment designed to test for pyroelectricity performed⁶ upon a rather large specimen of $\text{Rb}_3\text{TlBr}_6 \cdot (8/7)\text{H}_2\text{O}$ gave a negative result.

Within the tetragonal cell we must place 14 Tl, 42 K, 84 Cl, and 28 O; evidently we must deal with a many-parameter structure. We find, however, that the x-ray data suffice to fix the positions of thallium, following which the introduction of a few reasonable assumptions suggested by chemical and structural considerations permits of the complete elucidation of a structure which leads to satisfactory agreement between calculated and observed intensities of x-ray reflections.

Without giving the argument in detail, the relatively very strong intensities observed for all

reflections from (001) and (100) with $n/4$ integral seem to require the following arrangement⁷ of thallium atoms: 2 Tl in $2(a)$, 000; etc., 4 Tl in $4(c)$, $0\frac{1}{2}0$, $\frac{1}{2}00$; etc., 8 Tl in $8(f)$, $\frac{1}{4}\frac{1}{4}\frac{1}{4}$; $\frac{1}{4}\frac{3}{4}\frac{1}{4}$; $\frac{3}{4}\frac{1}{4}\frac{1}{4}$; $\frac{3}{4}\frac{3}{4}\frac{1}{4}$, etc. Except for the unoccupied positions $00\frac{1}{2}$; $\frac{1}{2}\frac{1}{2}0$, the thallium atoms are arranged at the points of a body centered tetragonal lattice with $a_0' = (15.84/2)\text{\AA}$, $c_0' = (18.005/2)\text{\AA}$.

The ratio of the univalent radii,⁸ $r_{\text{Tl}^{+++}}/r_{\text{Cl}^{-}}$, is 0.635, indicating a coordination number toward chlorine for thallium of six, or possibly of eight. The symmetry of the positions in question in every case rules out the structurally improbable coordination number of seven. The thallium atoms are placed too far apart to permit of sharing of polyhedron elements, so that a coordination number of eight can occur throughout only if water in addition to chlorine is coordinated. Symmetry requirements make this at least very improbable, and the evidence strongly indicates that TlCl_6^{3-} octahedra are structural units.

In $\text{Cs}_3\text{Tl}_2\text{Cl}_9$, thallium shows a coordination number toward chlorine of six. The existence of the $\text{Tl}_2\text{Cl}_3^{3-}$ complex together with the Tl—Cl separations which are found therein seem to show definitely that the Tl—Cl linkage is primarily covalent rather than ionic in character. In $\text{K}_3\text{TlCl}_6 \cdot 2\text{H}_2\text{O}$ we assume the existence of regular TlCl_6^{3-} octahedra with Tl—Cl = 2.55Å. This is obtained by adding the "octahedral" radius⁹ of Tl^{III} to the "normal" radius of Cl; this value we regard as more reliable than either of the experimentally determined values, 2.54 and 2.66Å, obtained from $\text{Cs}_3\text{Tl}_2\text{Cl}_9$, because of the shared face in the $\text{Tl}_2\text{Cl}_3^{3-}$ complex. The sum of the ionic radii, 2.76Å, is 0.21Å larger than the covalent Tl—Cl separation which we use here.

The TlCl_6^{3-} octahedra of $2(a)$ and $4(c)$ are required by the symmetry of those positions to assume one of two discrete orientations which differ by a rotation of 45° about c . The octahedra of $8(f)$ may in addition have an arbitrary rotation about the twofold axes which are perpendicular to $\{110\}$. These restrictions are sufficient to permit us to select reasonable positions not only

⁴ Int. Crit. Tab. 1, 156 (1926).

⁵ Ashbury and Yardley, *Tabulated Data for the Examination of the 230 Space Groups by Homogeneous X-Rays*, Phil. Trans. 224, 221–57 (1924).

⁶ See A. J. P. Martin, Min. Mag. 22, 519 (1931).

⁷ R. W. G. Wyckoff, *The Analytical Expression of the Results of the Theory of Space Groups*, second edition (Carnegie Inst. of Wash., 1930), p. 99.

⁸ Linus Pauling, J. Am. Chem. Soc. 49, 765 (1927).

⁹ Pauling and Huggins, Zeits. f. Krist. 87, 205 (1934).

for the potassium ions but also for the water molecules, leading ultimately to the complete determination of the structure. The parameter values given are the result of careful consideration of the many interatomic distances involved, and lead to satisfactory agreement between calculated and observed intensities.

The octahedra with centers in 2(a) have

4 Cl_I in 4(e): 00*u*; etc., with $u_I = 0.142$.

8 Cl_{II} in 8(i): $u00$; etc., with $u_{II} = 0.161$.

The octahedra with centers in 4(c) have

8 Cl_{III} in 8(g): $0\frac{1}{2}u$; etc., with $u_{III} = 0.142$.

16 Cl_{IV} in 16(l): $uv0$; etc., with $u_{IV} = 0.386$, $v_{IV} = 0.114$.

The octahedra with centers in 8(f) have

16 Cl_V in 16(m): $u\bar{u}v$; etc., with $u_V = 0.181$, $v_V = 0.362$.

16 Cl_{VI} in 16(n): $u\bar{u}v$; etc., with $u_{VI} = 0.160$, $v_{VI} = 0.163$.

16 Cl_{VII} in 16(k): u , $u + \frac{1}{2}$, $\frac{1}{2}$; etc., with $u_{VII} = 0.364$.

Potassium positions are

2 K_I in 2(b): $00\frac{1}{2}$; $\frac{1}{2}0$.

8 K_{II} in 8(h): $xx0$; etc., with $x_{II} = 0.214$.

16 K_{III} in 16(n): $0xy$; etc., with $x_{III} = 0.295$, $y_{III} = 0.132$.

16 K_{IV} in 16(n): $0xy$; etc., with $x_{IV} = 0.293$, $y_{IV} = 0.376$.

Oxygen positions are

4 O_I in 4(e): $00l$; etc., with $l_I = 0.347$.

8 O_{II} in 8(j): $s0\frac{1}{2}$; etc., with $s_{II} = 0.173$.

16 O_{III} in 16(n): $0st$; etc., with $s_{III} = 0.157$, $t_{III} = 0.276$.

The structure is seen to have nineteen determinable parameters.

In Table I we present the comparison between calculated and visually estimated intensities for several groups of reflections. The f values employed are those of Pauling and Sherman.¹⁰ No correction is included either for the decrease in intensity arising from the thermal vibrations of the atoms within the lattice or for absorption by the crystal; the latter is large enough so that only reflections with quite substantial structure factors are observed.

The agreement between calculated and observed intensities is quite generally satisfactory. For a structure of this complexity the calculated intensities are not much affected by rather substantial variations in the positions of the lighter atoms. We shall show, however, that this atomic arrangement is structurally very satisfactory; this fact together with the intensity data make it highly probable that the suggested structure is the true one.

One point about the intensity comparisons seems worthy of special mention. We notice that reflections from (001) and (100) with $n/4$ half-

TABLE I. Comparison of calculated with observed intensities.*

INTENSITY			INTENSITY		
(hkl)	Observed	Calculated	(hkl)	Observed	Calculated
002	<1	0.35	800	12	19.1
004	6	7.5	10·0·0	<1	3.9
006	3	7.5	12·0·0	4	7.6
008	45	60.0	14·0·0	0	2.2
0·0·10	0	0.1	16·0·0	2	8.2
0·0·12	6	11.3	18·0·0	0	2.0
0·0·14	<1	4.4	20·0·0	1	5.8
0·0·16	7	18.0	101	†	0.10
0·0·18	0	0.3	202	8	9.7
0·0·20	2	6.7	303	0	0.01
0·0·22	0	2.4	404	<1	0.73
0·0·24	2	8.9	505	0	0.07
0·0·26	0	0.03	606	4	13.0
0·0·28	0	4.4	707	0	0.42
200	<1	0.21	808	3	10.4
400	8	12.6	909	0	0.04
600	4	18.7	10·0·10	1.5	5.0

* Temperature factor not included.

† Not observed.

integral, e.g., (006) and (0·0·14), are observed to be weaker relative to reflections with $n/4$ integral than a comparison of their calculated intensities would indicate. The structure factor contains $14f_{T1}$ for $n/4$ integral, but only $2f_{T1}$ for $n/4$ half-integral; the main contributions to $S_{(006)}$ and $S_{(0·0·14)}$ are from chlorine and potassium. The decrease in atomic scattering powers arising from thermal agitation is very large for this structure, and, moreover, evidently should be much more marked for potassium and chlorine than for thallium atoms. Apparent discrepancies of the type observed are thus to be anticipated.

Crystals of $Rb_3TlBr_6 \cdot (8/7)H_2O$ were prepared according to the directions of Pratt.¹¹ Laue and oscillation data show the unit cell to be body centered tetragonal with $a_0 = 16.95$, $C_0 = 19.45$ Å, about, with D_{4h}^{17} as the probable space group. With 14 $Rb_3TlBr_6 \cdot (8/7)H_2O$ within the unit cell, the calculated density is 3.97 g/cm³, to be compared with the experimental¹ value 4.07 g/cm³. Upon the basis of quite meager analytical data, Pratt assigns the formula $Rb_3TlBr_6 \cdot H_2O$ to this compound, requiring the placing of 14 H_2O within the unit cell. Since his analysis actually indicates a somewhat higher proportion of water, and since, moreover, symmetry conditions do not permit of the placing of 14 H_2O within the structure which we have developed, we have decided

¹⁰ Pauling and Sherman, *Zeits. f. Krist.* **81**, 1 (1932).

¹¹ J. H. Pratt, *Am. J. Sci.* **149**, 397 (1895).

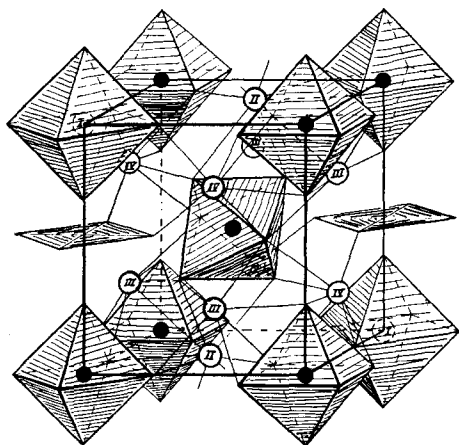


FIG. 1. One-eighth of the tetragonal unit cell of $K_3TiCl_6 \cdot 2 H_2O$. Thallium atoms are represented by closed blackened circles at the centers of octahedra whose vertices show the positions of chlorine atoms. Potassium ions are represented by open circles, the two larger octahedra being $K(H_2O)_6^+$. Water molecules of 16(n) are represented by the corners of the two squares (shown in perspective). Crystallographically distinct kinds of potassium ions and their coordination properties are indicated, respectively, by the attached labels and by the lines connecting circles with vertices of various polyhedra.

that the unit cell contains 16 H_2O (or perhaps more). This is discussed in detail later.

Using regular $TiBr_6^{3-}$ octahedra with a Ti-Br separation of 2.70Å, the following assignment of parameter values leads to generally satisfactory interatomic distances:

- The octahedra with centers in 2(a) have
 4 Br_I in 4(e): 00u; etc., with $u_I = 0.139$.
 8 Br_{II} in 8(i): u00; etc., with $u_{II} = 0.159$.
 The octahedra with centers in 4(c) have
 8 Br_{III} in 8(g): $0\frac{1}{2}u$; etc., with $u_{III} = 0.139$.
 16 Br_{IV} in 16(l): uv0; etc., with $u_{IV} = 0.387$, $v_{IV} = 0.113$.
 The octahedra with centers in 8(f) have
 16 Br_V in 16(m): $u\bar{u}v$; etc., with $u_V = 0.181$, $v_V = 0.360$.
 16 Br_{VI} in 16(n): $u\bar{u}v$; etc., with $u_{VI} = 0.161$, $v_{VI} = 0.165$.
 16 Br_{VII} in 16(k): u, u + $\frac{1}{2}$, $\frac{1}{2}$; etc., with $u_{VII} = 0.363$.
 Rubidium positions are
 2 Rb_I in 2(b): 00 $\frac{1}{2}$; $\frac{1}{2}$ 00.
 8 Rb_{II} in 8(h): xx0; etc., with $x_{II} = 0.214$.
 16 Rb_{III} in 16(n): 0xy; etc., with $x_{III} = 0.295$, $y_{III} = 0.132$.
 16 Rb_{IV} in 16(k): 0xy; etc., with $x_{IV} = 0.293$, $y_{IV} = 0.366$.
 Oxygen positions are
 16 O_I in 16(n): 0st; etc., with $s_I = 0.122$, $t_I = 0.400$.

Our intensity data are inadequate to permit of the detailed testing of this structure through a

comparison of calculated and observed intensities of x-ray reflections.

DISCUSSION OF THE STRUCTURE

The essential nature of the structure can be readily understood by reference to a pseudo unit (Fig. 1) of 1/2 the axial lengths and 1/8 the volume of the true tetragonal cell. Each face of this prism lies in a plane of symmetry; the other seven parts of the true unit may then be visualized without difficulty.

This pseudo unit, containing $1\frac{3}{4}$ molecules, is comparable with the two molecule body centered tetragonal unit of the ammonium fluoferrate structure.¹²

In the $K_3TiCl_6 \cdot 2 H_2O$, as opposed to the $(NH_4)_3FeF_6$ structure, two octahedra [2(b)] are missing, two octahedra [2(a)] are rotated through 45° about c, and 8 octahedra are rotated through 37.5° about the twofold axes perpendicular to {110}. The coordination around potassium ions in $K_3TiCl_6 \cdot 2 H_2O$ is very different from that around the analogous ammonium ions in $(NH_4)_3FeF_6$. Whereas in the latter structure $\frac{2}{3}$ of the NH_4^+ ions are closely surrounded by 12 F^- and the remaining $\frac{1}{3}$ by only 6 F^- , in $K_3TiCl_6 \cdot 2 H_2O$ 24 of the 42 K^+ ions are closely surrounded by 8 Cl^- , 16 K^+ by 7 Cl^- and 2 H_2O , and the remaining 2 K^+ by 6 H_2O . The structural relations to their surroundings of 40 of the 42 K^+ ions are entirely satisfactory, and, although less

TABLE II. Interatomic distances in $K_3TiCl_6 \cdot 2 H_2O$.

ATOM	NEIGHBORS	SEPARATION	ATOM	NEIGHBORS	SEPARATION
K _I	2 O _I , 4 O _{II}	2.75A	K _{IV}	1 O _{II}	2.90A
K _I	8 O _{III}	4.73	K _{IV}	1 O _{III}	2.80
K _I	8 Cl _V	4.75	Cl _I	4 Cl _{VI}	3.60
K _I	8 K _{IV}	5.15	Cl _I	4 O _{III}	3.46
K _{II}	2 Cl _{II}	3.49	Cl _{II}	4 Cl _{VI}	3.94
K _{II}	2 Cl _{IV}	3.16	Cl _{II}	2 Cl _{IV}	4.00
K _{II}	2 Cl _V	3.42	Cl _{III}	1 Cl _{III}	3.90
K _{II}	2 Cl _{VI}	3.18	Cl _{III}	4 Cl _{VII}	3.62
K _{III}	1 Cl _{II}	3.20	Cl _{IV}	2 Cl _V	4.20
K _{III}	1 Cl _{III}	3.26	Cl _{IV}	2 Cl _{VI}	4.80
K _{III}	2 Cl _{IV}	3.31	Cl _V	2 Cl _{VII}	4.60
K _{III}	2 Cl _{VI}	3.34	Cl _V	2 O _{II}	3.80
K _{III}	2 Cl _{VII}	3.21	Cl _V	2 O _{III}	3.28
K _{IV}	1 Cl _{III}	3.29	Cl _{VI}	2 O _{III}	3.25
K _{IV}	2 Cl _{IV}	3.23	Cl _{VII}	1 Cl _{VII}	3.96
K _{IV}	2 Cl _V	3.37	O _I	4 O _{II}	3.90
K _{IV}	2 Cl _{VII}	3.31	O _I	4 O _{III}	2.80

¹² R. W. G. Wyckoff, *The Structure of Crystals*, second edition (Chemical Catalog Co., New York, 1931), p. 307.

favorably placed, the remaining 2 K^+ are also in regions of negative potential. Each K^+ of 2(b) is surrounded by 6 H_2O at 2.75Å, 8 H_2O at 4.73Å, 8 Cl^- at 4.75Å, 8 K^+ at 5.15Å, and 10 Cl^- at still larger distances.

Our assignment of parameter values necessarily places each Tl at the center of a regular $TlCl_6$ octahedron with $Tl-Cl=2.55Å$, $Cl-Cl=3.61Å$. The closest distance of approach of two thallium atoms is 7.17Å. All other interatomic distances which bear directly upon the question of the stability of this structure are given in Table II.

The $K-Cl$ separation varies from 3.16 to 3.49 with an average value of 3.30Å, closely that to be expected for a coordination number of eight. Other interatomic distances are in equally good agreement with theory and past experience. Considered as a whole, the most striking feature of the structure is its compactness. Having first adjusted the values of potassium and chlorine parameters so as to make all $K-Cl$ separations satisfactory, it turns out that the potassium ions of 2(b) can coordinate no more than 6 H_2O , and, moreover, that the 28 H_2O can be placed in only one way; there is no room in the structure for additional water. The apparently accurate chemical analysis² is entirely consistent with this finding.

Since dimensional relations within the structure permit the coordination of no more than 6 H_2O by K^+ , we may not conclude that this represents the normal degree of hydration of the potassium ion. In general, and especially in the crystalline state, a higher degree of hydration is to be anticipated.

The assumption of regular $TlCl_6^{3-}$ octahedra with $Tl-Cl=2.55Å$ leads to $Cl-Cl=3.61Å$, just the ionic diameter of Cl^- . Small departures from regularity in the octahedra, not materially affect-

ing interatomic distances throughout, are not improbable.

If the $Tl-Cl$ separation were from 0.1 to 0.2Å larger than that assumed, we should find the problem of adjusting parameter values so as to obtain generally satisfactory interatomic distances definitely embarrassing, and probably impossible. As already pointed out,¹ the existence in $Cs_3Tl_2Cl_9$ of $Tl_2Cl_9^{3-}$ double octahedra with shared faces constitutes convincing evidence that the bond type is largely covalent rather than ionic in character. The structures of both $Cs_3Tl_2Cl_9$ and $K_3TlCl_6 \cdot 2H_2O$ indicate that thallic thallium tends to form six stable covalent bonds with chlorine. It is probable that the $Tl-Cl$ separation in the $TlCl_6^{3-}$ group does not vary from the value 2.55Å by more than a few hundredths of an Angstrom unit.

Values of the $Rb-Br$ separation in $Rb_3TlBr_6 \cdot (8/7)H_2O$ range from 3.40 to 3.70Å, the average being 3.54Å. The only critical contacts between bromine atoms of different octahedra are 3.90Å for $Br_{I1}-Br_{VI1}$ and 3.93Å for $Br_{IV1}-Br_{VII1}$, to be compared with 3.90Å for the ionic diameter. In $K_3TlCl_6 \cdot 2H_2O$ it is dimensionally impossible for the potassium ions of 2(b) to coordinate more than 6 H_2O , but in the bromothallate each rubidium of 2(b) can coordinate at least 8 H_2O . We find $Rb_{I1}-O_1=2.86Å$, $Rb_{IV1}-O_1=2.97Å$, $O_1-O_1=2.92$ and $3.89Å$, $O_1-Br_{VI1}=3.31Å$. With some variations from the parameter values given, it might be possible to add either 4 H_2O in 4(e) or 8 H_2O in 8(h) to give rubidium effectively a coordination number of either ten or twelve, respectively. The latter possibility appears the more probable from a dimensional standpoint.

Except for the degree of hydration of the alkali ions of 2(b), crystals of $K_3TlCl_6 \cdot 2H_2O$ and $Rb_3TlBr_6 \cdot (8/7)H_2O$ are truly isomorphous.