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THE CRYSTAL STRUCTURE OF SYNTHETIC RADTKEITE, Hg_3S_2ClI

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ABSTRACT

The crystal structure of the artificial analogue of the rare mineral radtkeite, $Hg^{2+}{}_3S_2ClI$ [monoclinic, space group $C2/m$, $Z = 8$, a 16.827(4), b 9.117(1), c 13.165(5) Å, β 130.17(2)°, V 1543.2(7) Å^3] has been solved by direct methods, and refined to an R index of 5.27%, on the basis of 1498 unique reflections ($R_{int} = 0.0254$) measured with Mo$K\alpha$ radiation on a CAD-4 automated diffractometer. The transformation $\vec{a}_{orth}' = \vec{a}_m$, $\vec{b}_{orth}' = \vec{a}_m + 2\vec{c}_m = 20.120(4)$ Å, and $\vec{c}_{orth}' = \vec{b}_m$ produces a pseudo-orthorhombic F-cell, in which $\alpha_o' = \beta_o' = 90°$, and γ_o' differs slightly from 90° (89.55°). Close agreement of these cell dimensions with those reported for natural radtkeite confirms the identity of these compounds, as does the good match between calculated X-ray-diffraction patterns and the powder-diffraction pattern of natural radtkeite. The structure contains five independent mercury atoms; each Hg^{2+} is covalently bonded to two sulfur atoms at a distance of 2.240(6)–2.474(8) Å; the angles S(2)–Hg(1)–S(2)' and S(1)–Hg(3)–S(1)' equal 177.9(4) and 180.0(3)°, respectively. The angles S(2)–Hg(5)–S(1) [146.1(2)°], S(1)–Hg(4)–S(1)' [161.8(3)°] and S(2)–Hg(2)–S(2)' [164.3(3)°] deviate greatly from linearity. Corrugated $[Hg_{12}S_8]_{\infty\infty}$ layers are parallel to (001) in the structure. Halogen atoms are located inside and between the $[Hg_{12}S_8]_{\infty\infty}$ layers, at Hg–Cl and Hg–I distances of 2.783(7)–2.961(6) and 3.167(4)–3.231(2) Å, respectively.

Keywords: radtkeite, synthetic, sulfohalide of mercury, structure determination.

SOMMAIRE

Nous avons résolu la structure cristalline de l'analogue synthétique de la radtkéite, $Hg^{2+}{}_3S_2ClI$ [monoclinique, groupe spatial $C2/m$, $Z = 8$, a 16.827(4), b 9.117(1), c 13.165(5) Å, β 130.17(2)°, V 1543.2(7) Å^3], par méthodes directes, et nous l'avons affiné jusqu'à un résidu R de 5.27%, en utilisant 1498 réflexions uniques ($R_{int} = 0.0254$) mesurées avec rayonnement Mo$K\alpha$ et un diffractomètre CAD-4 automatisé. La transformation $\vec{a}_{orth}' = \vec{a}_m$, $\vec{b}_{orth}' = \vec{a}_m + 2\vec{c}_m = 20.120(4)$ Å, et $\vec{c}_{orth}' = \vec{b}_m$ produit une maille pseudo-orthorhombique à F centré, dans laquelle $\alpha_o' = \beta_o' = 90°$, et γ_o' diffère légèrement de 90° (89.55°). Une concordance étroite entre ces dimensions réticulaires et celles pour la radtkéite holotypique confirme l'identité de ces composés, tout comme la grande corcordance dans les spectres de diffraction X, calculé d'une part et celui de la radtkéite naturelle. La structure contient cinq atomes indépendants de mercure; chaque atome Hg^{2+} est en liaison covalente avec deux atomes de soufre à une distance de 2.240(6)–2.474(8) Å; les angles S(2)–Hg(1)–S(2)' et S(1)–Hg(3)–S(1)' sont 177.9(4) et 180.0(3)°, respectivement. Les angles S(2)–Hg(5)–S(1) [146.1(2)°], S(1)–Hg(4)–S(1)' [161.8(3)°] et S(2)–Hg(2)–S(2)' [164.3(3)°] devient largement de la linéarité. Des couches ondulantes de $[Hg_{12}S_8]_{\infty\infty}$ sont parallèles à (001) dans la structure. Les atomes de halogène sont situés à l'intérieur et entre les couches $[Hg_{12}S_8]_{\infty\infty}$, à des distances Hg–Cl et Hg–I de 2.783(7)–2.961(6) et 3.167(4)–3.231(2) Å, respectivement.

(Traduit par la Rédaction)

Keywords: radtkéite, synthétique, sulfohalogénure de mercure, détermination de la structure.

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INTRODUCTION

The new mercury sulfohalide mineral radtkeite, Hg_3S_2ClI, was first described by McCormack *et al.* (1991). It has only been found at the McDermitt mercury deposit, Nevada, U.S.A. Radtkeite is closely associated with cinnabar and corderoite in strongly altered host-rocks predominantly composed of montmorillonite, kaolinite, K-feldspar of the adularia habit, opal, cristobalite, and quartz, among others. Other rare mercury minerals that occur at the McDermitt deposit are calomel, kleinite, eglestonite, native mercury, and possibly mosesite.

Radtkeite occurs as submicrometric grains, irregular masses, and euhedral crystals up to 10 μm wide by 30 μm long. Tabular prismatic crystals are the most abundant. They supposedly are hypogene and formed by reaction of chloride–iodide-bearing hydrothermal solutions with cinnabar and corderoite during late stages of mineralization under near-surface conditions.

Physical and optical properties, composition, and X-ray characteristics of natural and synthetic specimens were studied, but the structure of the mineral was not solved at that time. It was determined that radtkeite is orthorhombic, with proposed space-groups *Fmmm*, *F*222, or *Fmm*2. The unit-cell parameters reported are: *a* 16.85(1), *b* 20.27(2), *c* 9.133(2) Å, *V* 3119.4(5) Å^3, *Z* = 16.

We report here on an investigation of its structure, conducted on synthetic radtkeite.

EXPERIMENTAL

As natural samples of radtkeite were unavailable, we synthesized its analogue by a procedure mentioned by McCormack *et al.* (1991). The initial substances were artificial red mercury sulfide HgS, mercury halides $HgCl_2$, and HgI_2, previously prepared and taken in appropriate proportions to obtain Hg_3S_2ClI. Single crystals and aggregates were grown during this experiment at 220°C. Typical yellow-orange single crystals produced by this method have mostly elongate, tabular and prismatic forms (Fig. 1), and are very similar to natural radtkeite. Physical and optical properties of our specimens are similar to those reported by McCormack *et al.* (1991).

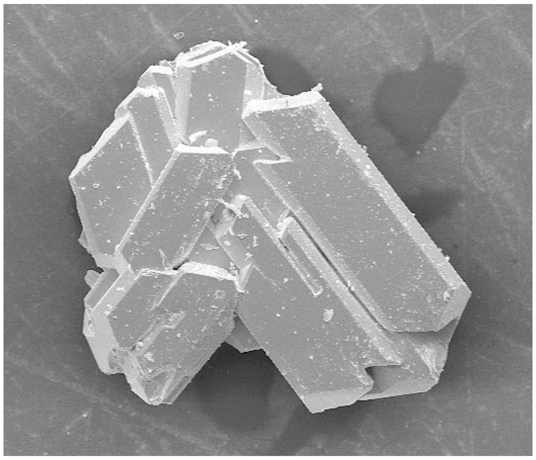

FIG. 1. SEM photomicrograph of an aggregate of crystals of the synthetic analogue of radtkeite. The aggregate is 0.58 mm across at its widest.

Chemical analyses of this specimen and other crystals were carried out on a CAMEBAX–MICRO electron microprobe. Artificial HgS (Hg*M*α, S*K*α lines), HgI_2 (I*L*α) and natural calomel Hg_2Cl_2 (Cl*K*α) were used as standards under an accelerating voltage of 20 kV, a beam current of 16 nA, and a beam diameter of 5 μm. The mean composition of the substance, derived from nine analyses, is Hg 73.99, S 6.80, Cl 4.72, I 15.05 wt% (Table 1). The empirical formula, calculated on the basis of a total of seven atoms, is $Hg_{3.10}S_{1.78}Cl_{1.12}I_{1.00}$, which is very close to that calculated for an average composition for all synthetic specimens, $Hg_{3.12}S_{1.78}Cl_{1.12}I_{0.98}$.

We used a prismatic crystal having dimensions of 0.08 × 0.12 × 0.32 mm for X-ray investigations of the structure. Unit-cell parameters were refined, and intensity data were obtained using an Enraf–Nonius CAD4 diffractometer operating at room temperature and using graphite-monochromated Mo*K*α radiation. Data were corrected for Lorentz and polarization effects. Absorption corrections were applied using the X–RED package of programs (X–RED 1999). An analysis of intensity data showed that monoclinic symmetry is preferable to an orthorhombic one (R_{int} for monoclinic symmetry equals to 2.54%, whereas R_{int} for orthorhombic symmetry is about 22.3%). Attempts to refine the structure within orthorhombic groups *Fmm*2, *Fmmm*, and *F*222 were unsatisfactory; therefore, final refinement was performed within the space group *C*2/*m*. The structure was solved by direct methods using SIR97 (Altomare *et al.* 1999) and refined anisotropically by a

TABLE 1. ELECTRON-MICROPROBE DATA FOR THE CRYSTALS OF SYNTHETIC Hg_3S_2ClI

	1	2	3	4	5	6	7	8	9
Hg wt %	73.49	73.85	74.91	73.70	74.85	73.78	74.40	74.06	74.13
S	6.96	6.83	6.23	7.18	6.88	7.05	6.66	6.19	6.75
Cl	4.90	4.78	4.66	4.55	4.95	4.24	4.93	4.53	4.69
I	14.91	15.59	15.12	14.59	14.35	13.94	15.03	14.87	14.80
Total	100.27	101.06	100.92	100.02	101.02	99.01	101.01	99.66	100.37

Note: columns 1–4: results of analyses made on the crystal chosen for the X-ray investigation (after the refinement). Columns 5–8: results of analyses made on other crystals (one analysis each). Column 9: the mean values for all specimens.

full-matrix least-squares technique using the SHELX97 program package (Sheldrick 1998). Selected experimental data are given in Table 2, final atomic coordinates and thermal parameters are given in Table 3, and selected bond-lengths and angles are given in Table 4. A table of structure factors is available from the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada.

DESCRIPTION OF THE STRUCTURE

The structure of synthetic radtkeite contains five independent atoms of mercury. Each Hg^{2+} atom is covalently bonded to two sulfur atoms at a distance of 2.240(6)–2.474(8) Å, and the angles S(2)–Hg(1)–S(2)' and S(1)–Hg(3)–S(1)' are equal to 177.9(4) and 180.0(3)°, respectively, as is typical of Hg^{2+} compounds (Aurivillius 1965). It is noteworthy that the S(2)–Hg(5)–S(1) [146.1(2)°], S(1)–Hg(4)–S(1)' [161.8(3)°] and S(2)–Hg(2)–S(2)' [163.4(3)°] angles deviate greatly from linearity.

Each S^{2-} is covalently bonded to three mercury atoms at distances of 2.240(6)–2.474(8) Å. The Hg–S–Hg angle varies from 94.7(2) to 102.9(2)°. As a result, the structure contains linear covalently bonded S–Hg–S' groups and SHg3 "umbrellas", which are similar to those in mercury chalcogenide halide structures of the composition $Hg_3X_2Hal_2$ (X = S, Se, Te; Hal = Cl, Br, I) (Aurivillius 1967, Beck & Hedderich 2000, Borisov *et al.* 1999, Ďurovič 1968, Lyachovtskaya *et al.* 1989, Puff & Küster 1962a, b, Voroshilov *et al.* 1995, 1996a, b). These units form corrugated $[Hg_{12}S_8]_{\infty\infty}$ layers that are parallel to (001). In these layers, five out of six of the Hg–S bonds form closed $[Hg_4S_4]$ rings having two orientations, and one out of six links these rings *via* Hg–S–Hg bridges to form the layer (Fig. 2). Analogous Hg–X layers occur in the structures of γ–$Hg_3S_2Cl_2$ (Ďurovič 1968), β–$Hg_3S_2Br_2$ (Voroshilov *et al.* 1996a), $Hg_3Se_2Br_2$ (Voroshilov *et al.* 1995), synthetic $Hg_3S_2Cl_{1.5}Br_{0.5}$ – (II) (Borisov *et al.* 1999), and possibly in the mineral kenhsuite (McCormack & Dickson 1998).

TABLE 2. CRYSTAL DATA FOR Hg_3S_2ClI

a (Å)	16.827(4)	D_{calc} (g/cm^3)	7.130
b (Å)	9.117(1)	μ (mm^{-1})	64.32
c (Å)	13.165(5)	Unique reflections	5613
β (°)	130.17(2)	Unique $F_o > 4\sigma_F$	1444
V (Å^3)	1543.2(7)	Final R $F_o > 4\sigma_F$	0.0527
Space group	$C2/m$		
Z	8		

$R = \Sigma(|F_o| - |F_c|) / \Sigma|F_o|$

Halogen atoms are located inside and between the $[Hg_{12}S_8]_{\infty\infty}$ layers, and have Hg–Cl and Hg–I distances in the ranges 2.783(7)–2.961(6) and 3.167(4)–3.311(4) Å, respectively. As in the known structures of other sulfohalides of mercury having composition $Hg_3X_2Hal_2$ (X = S, Se, Te; Hal = Cl, Br, I), the halogen atoms form a primitive pseudocubic sublattice with sulfur atoms at its center and mercury atoms in its face centers (Fig. 3). This arrangement results in stable radicals having covalent Hg–S bonds that cross the halogen lattice (Borisov *et al.* 2001). These halogen atoms, give the Hg(1)–Hg(5) atoms a distorted octahedral coordination (Fig. 4).

The perfect cleavage $\{010\}_{orth}$ for the F-cell (McCormack *et al.* 1991) coincides both with the plane of the $[Hg_{12}S_8]_{\infty\infty}$ layer and one of the close square nets of a primitive pseudocubic sublattice of halogen atoms (Borisov *et al.* 2001). In the monoclinic C-cell, the perfect cleavage is the $\{001\}_m$ plane. The very good cleavages $\{001\}_{orth}$ and $\{100\}_{orth}$ are attributed to two other close square nets of halogen atoms. In the C-cell, these cleavages are the $\{010\}_m$ and $\{201\}_m$ planes, respectively. Some Hg–S bonds between the strongest $[Hg_{12}S_8]$ units of the layer are broken upon being shifted along these planes.

DISCUSSION

McCormack *et al.* (1991) gave the proposed space groups *Fmmm*, *F*222, *Fmm*2 (orthorhombic), and the unit-cell parameters, *a* 16.85(1), *b* 20.27(2), *c* 9.133(2)

TABLE 3. ATOM COORDINATES AND DISPLACEMENT PARAMETERS (Å^2) FOR RADTKEITE

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Hg(1)	0	0.2270(2)	-0.5000	0.027(1)	0.024(1)	0.026(1)	0	0.017(1)	0
Hg(2)	0.1510(1)	0.5000	-0.2535(2)	0.033(1)	0.031(1)	0.030(1)	0	0.020(1)	0
Hg(3)	-0.2500	0.2500	-0.5000	0.028(1)	0.031(1)	0.029(1)	-0.001(1)	0.019(1)	-0.001(1)
Hg(4)	-0.1405(1)	0.5000	-0.2342(2)	0.045(1)	0.040(1)	0.045(1)	0	0.031(1)	0
Hg(5)	0.0248(1)	0.2160(2)	-0.2048(1)	0.045(1)	0.047(1)	0.046(1)	0.000(1)	0.029(1)	0.000(1)
S(1)	-0.1475(5)	0.2331(8)	-0.2688(6)	0.021(3)	0.018(4)	0.030(3)	0.003(3)	0.016(3)	0.003(3)
S(2)	0.1234(5)	0.2315(9)	-0.2782(6)	0.024(3)	0.032(5)	0.029(4)	-0.001(4)	0.016(3)	0.004(3)
I(1)	-0.1245(2)	0.5000	0.0126(3)	0.033(2)	0.035(2)	0.033(2)	0	0.020(1)	0
I(2)	-0.3936(2)	0	-0.5269(3)	0.040(2)	0.032(2)	0.041(2)	0	0.027(2)	0
Cl(1)	0.1126(8)	0	-0.0101(10)	0.042(6)	0.026(6)	0.030(6)	0	0.028(5)	0
Cl(2)	0.1299(8)	0	-0.5162(11)	0.037(6)	0.042(7)	0.040(6)	0	0.031(5)	0

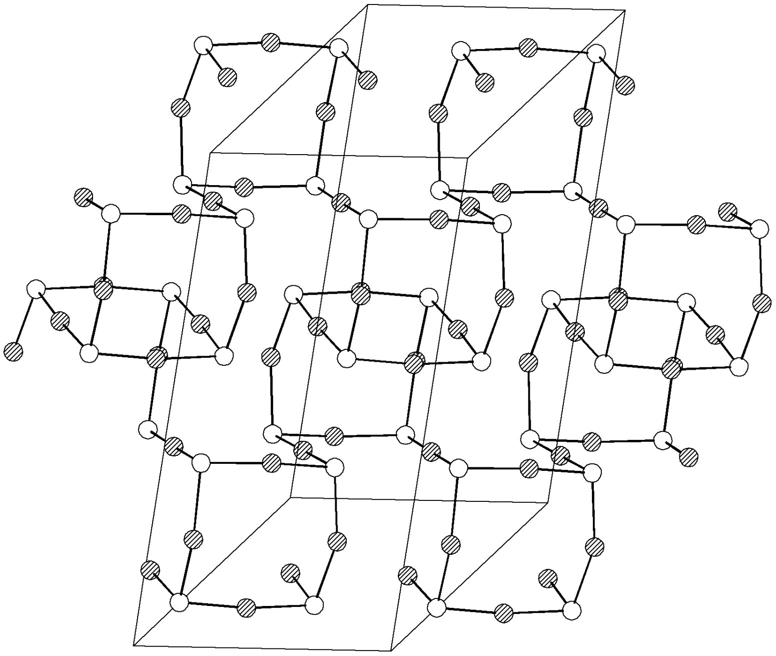

FIG. 2. The Hg–S two-dimensional layer in the unit cell of $Hg_3S_2Cl_{1.0}I_{1.0}$.

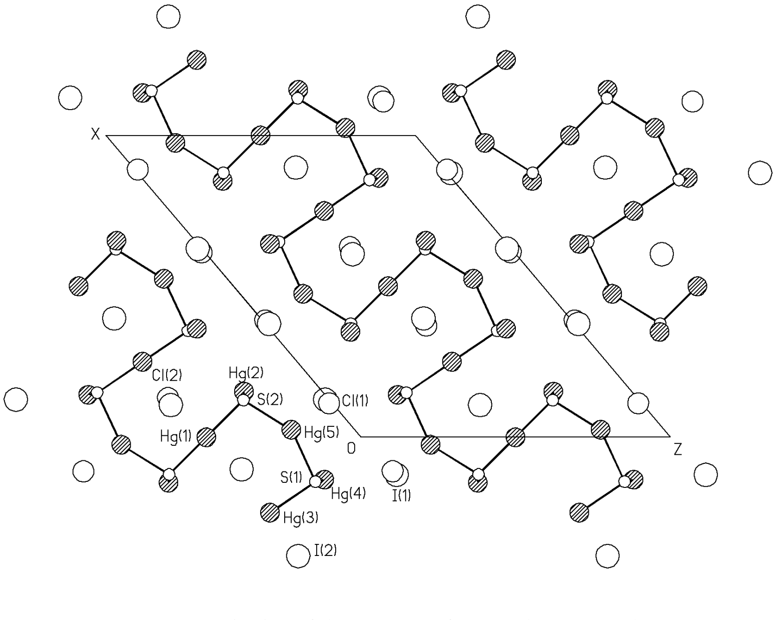

FIG. 3. Projection of the structure of $Hg_3S_2Cl_{1.0}I_{1.0}$ onto the plane (010).

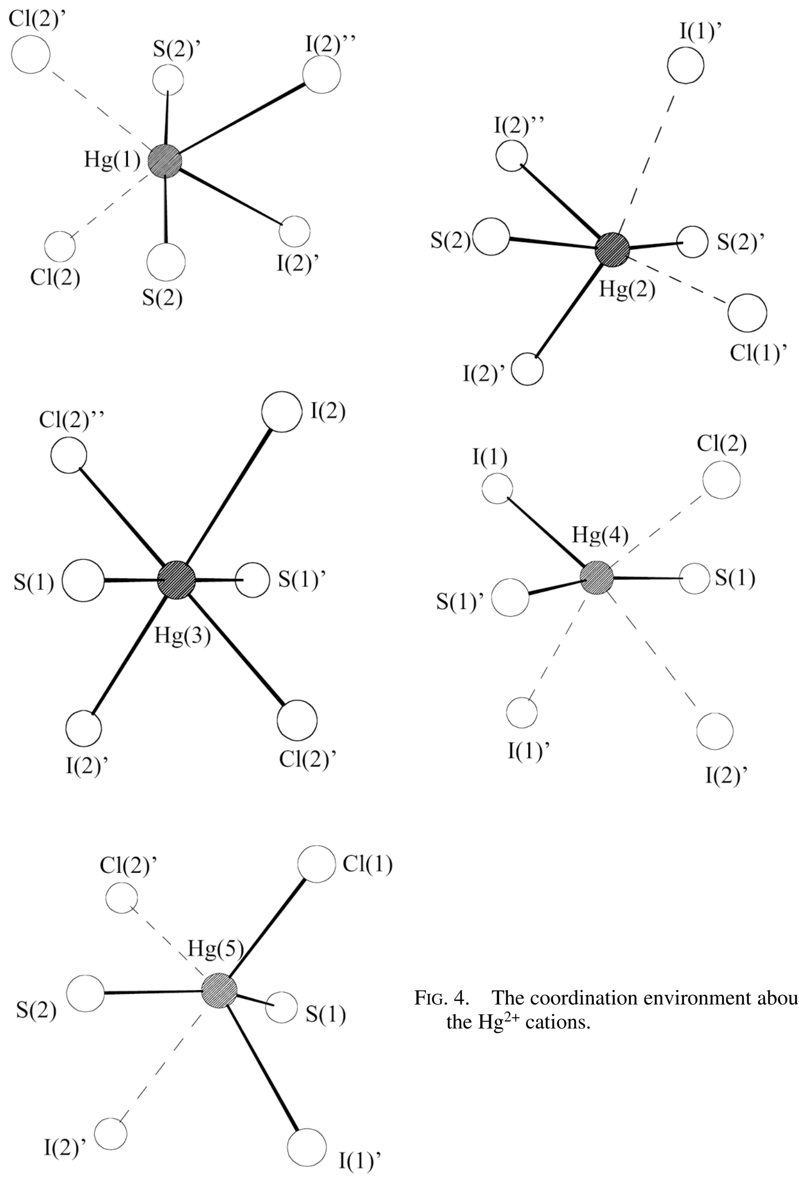

FIG. 4. The coordination environment about the Hg^{2+} cations.

Å, $Z = 16$, for radtkeite. Single-crystal X-ray analysis of the structure of the synthetic analogue reveals a monoclinic $C2/m$ symmetry with the following standard unit-cell parameters a_m 16.827(4), b_m 9.117(1), c_m 13.165(5) Å, β 130.17(2)°. The $\vec{a}_{\text{orth}}' = \vec{a}_{\text{m}}$, $\vec{b}_{\text{orth}}' = \vec{a}_{\text{m}} + 2\vec{c}_{\text{m}} =$ 20.120(4) Å, $\vec{c}_{\text{orth}}' = \vec{b}_{\text{m}}$ transition produces a pseudo-orthorhombic F-cell, in which $\alpha_{\text{orth}}' = \beta_{\text{orth}}' = 90°$, and γ_{orth}' slightly differs from 90° (89.55°) (Fig. 5). The close agreement of these cell dimensions with those reported by McCormack *et al.* (1991) confirms the identity of our compounds; also our calculated the powder X-ray-diffraction pattern (Table 5) matches the powder-diffraction pattern of natural radtkeite, as obtained by them.

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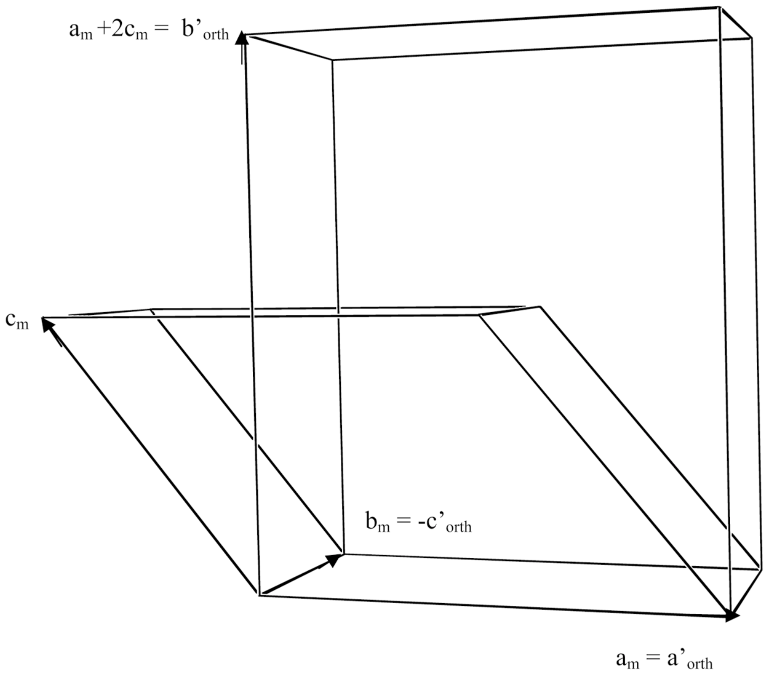

FIG. 5. The relation between monoclinic (a_m, b_m, c_m) and "orthorhombic" (a'_{orth}, b'_{orth}, c'_{orth}) unit cells in the structure of synthetic analogue of radtkeite.

TABLE 4. INTERATOMIC DISTANCES (Å) AND ANGLES (°) FOR RADTKEITE

Hg(1)-S(2) × 2	2.240(6)	Hg(3)-Cl(2) × 2	2.961(6)
Hg(2)-S(2) × 2	2.474(8)	Hg(5)-Cl(1)	2.783(7)
Hg(3)-S(1) × 2	2.343(6)	Hg(1)-I(2) × 2	3.216(2)
Hg(4)-S(1) × 2	2.464(7)	Hg(2)-I(2)#3	3.167(4)
Hg(5)-S(2)	2.403(7)	Hg(2)-I(2)#2	3.311(4)
Hg(5)-S(1)	2.447(6)	Hg(3)-I(2) × 2	3.171(2)
		Hg(4)-I(1)	3.083(4)
		Hg(5)-I(1)#7	3.231(2)
S(2)-Hg(1)-S(2)#1	177.9(4)	Hg(3)-S(1)-Hg(5)	99.7(2)
S(2)-Hg(2)-S(2)#4	163.4(3)	Hg(3)-S(1)-Hg(4)	94.7(2)
S(1)-Hg(3)-S(1)#2	180.0(3)	Hg(5)-S(1)-Hg(4)	95.4(2)
S(1)-Hg(4)-S(1)#4	161.8(3)	Hg(1)-S(2)-Hg(5)	102.9(2)
S(2)-Hg(5)-S(1)	146.1(2)	Hg(1)-S(2)-Hg(2)	97.3(3)
		Hg(5)-S(2)-Hg(2)	97.2(3)

Symmetry transformations used to generate equivalent atoms:
#1 –*x*, *y*, –*z*–1
#2 –*x*–½, –*y*+½, –*z*–1
#3 *x*+½, *y*+½, *z*
#4 *x*, –*y*+1, *z*
#5 –*x*, –*y*, –*z*–1
#6 *x*–½, *y*+½, *z*
#7 –*x*, –*y*+1, –*z*
#8 –*x*, *y*, –*z*
#9 *x*–½, *y*–½, *z*
#10 –*x*–½, *y*–½, –*z*–1
#11 *x*, –*y*, *z*
#12 *x*+½, *y*–½, *z*

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TABLE 5. POWDER X-RAY-DIFFRACTION DATA FOR SYNTHETIC Hg_3S_2ClI AND NATURAL RADTKEITE

hkl (m)	*hkl* (orth)	$d_{synth.}$	$I_{synth.}$	*d* Rdk*	I Rdk*
0 0 1	0 2 0	10.0594	6.69	10.11	1
1 1 0	1 1 1	7.4371	11.93	7.50	1
$\bar{2}$ 0 2	$\bar{2}$ 2 0	6.4788	15.77	6.49	8
2 0 0	2 2 0	6.4287	32.02		
$\bar{1}$ 1 2	$\bar{1}$ 3 1	5.1531	14.05		
$\bar{3}$ 1 2	$\bar{3}$ 1 1	4.6550	45.93	4.66	6
0 2 0	0 0 2	4.5585	2.71		
$\bar{2}$ 0 3	$\bar{2}$ 4 0	4.3321	5.29	4.34	4
2 0 1	2 4 0	4.3022	8.38		
$\bar{4}$ 0 2		4.2066	2.50		
0 2 1	0 2 2	4.1521	63.82	4.15	18
$\bar{4}$ 0 3	$\bar{4}$ 2 0	3.8919	47.90		
3 1 0	3 3 1	3.8786	45.52	3.90	41
$\bar{4}$ 0 1	$\bar{4}$ $\bar{2}$ 0	3.8701	47.60		
$\bar{2}$ 2 2	$\bar{2}$ 2 2	3.7281	41.44	3.73	22
2 2 0	2 2 2	3.7185	21.91		
1 1 2	1 5 1	3.5907	11.49	3.65	4
0 0 3	0 6 0	3.3531	15.43	3.38	9
$\bar{2}$ 2 3	$\bar{2}$ 4 2	3.1402	5.20	3.15	6
2 2 1	2 4 2	3.1288	4.50		
$\bar{4}$ 2 2	$\bar{4}$ 0 2	3.0915	3.00	3.10	7
$\bar{3}$ 1 4	$\bar{3}$ 5 1	3.0878	31.74		
$\bar{4}$ 2 3	$\bar{4}$ 2 2	2.9599	11.19	2.96	24
1 3 0	1 1 3	2.9575	28.21		
$\bar{4}$ 2 1	$\bar{4}$ $\bar{2}$ 2	2.9503	14.21		
$\bar{1}$ 3 2	$\bar{1}$ 3 3	2.7328	10.09		
$\bar{6}$ 0 4	$\bar{6}$ 2 0	2.7069	28.98	2.71	44
0 2 3	0 6 2	2.7011	52.04		
$\bar{6}$ 0 2	$\bar{6}$ $\bar{2}$ 0	2.6959	20.83		
$\bar{4}$ 2 4	$\bar{4}$ 4 2	2.6406	100.00	2.64	100
$\bar{4}$ 0 5	$\bar{4}$ 6 0	2.6322	2.13		
4 2 0	4 4 2	2.6270	99.04		
$\bar{2}$ 2 4	$\bar{2}$ 6 2	2.5766	15.10	2.58	29
2 2 2	2 6 2	2.5671	7.29		
0 0 4	0 8 0	2.5148	61.53	2.53	28
$\bar{3}$ 3 3	$\bar{3}$ 3 3	2.4854	2.97	2.482	5
3 1 2	3 7 1	2.4555	4.55		
$\bar{2}$ 0 5	$\bar{2}$ 8 0	2.4147	3.60	2.423	4
$\bar{1}$ 3 3	$\bar{1}$ 5 3	2.4019	3.49		
1 3 2	1 5 3	2.3986	8.13		
0 4 0	0 0 4	2.2793	51.84	2.281	26
$\bar{7}$ 1 2	$\bar{7}$ $\bar{3}$ 1	2.1910	3.70		
$\bar{4}$ 0 6		2.1660	1.76		
$\bar{6}$ 0 6	$\bar{6}$ 6 0	2.1596	7.28	2.164	10
$\bar{6}$ 2 1		2.1521	1.48		
1 1 4	1 9 1	2.1512	2.24		
4 0 2	4 8 0	2.1511	3.78		
6 0 0	6 6 0	2.1429	3.70	2.144	7
$\bar{5}$ 3 4	$\bar{5}$ 3 3	2.1412	3.87		
$\bar{8}$ 0 4	$\bar{8}$ 0 0	2.1033	31.88	2.107	18
$\bar{1}$ 3 4	$\bar{1}$ 7 3	2.0737	3.13		
1 3 3	1 7 3	2.0708	2.19	2.072	3
$\bar{3}$ 1 6	$\bar{3}$ 9 1	2.0299	2.64	2.024	3
$\bar{4}$ 4 3	$\bar{4}$ 8 4	1.9668	9.55		
$\bar{4}$ 4 1	$\bar{4}$ $\bar{2}$ 4	1.9640	9.04	1.962	13
$\bar{4}$ 2 6	$\bar{4}$ 8 2	1.9564	4.96		
3 3 2	3 9 3	1.9533	2.17		
4 2 2	4 8 2	1.9454	3.52		
$\bar{8}$ 2 4	$\bar{8}$ 0 2	1.9098	3.65	1.916	4
$\bar{8}$ 2 5	$\bar{8}$ 2 2	1.8788	6.14	1.880	11
$\bar{7}$ 3 4	$\bar{7}$ 1 3	1.8782	11.90		
$\bar{8}$ 2 3	$\bar{8}$ $\bar{2}$ 2	1.8738	4.17		
6 0 1		1.8650	1.39		
0 2 5	0 10 2	1.8406	3.30		
$\bar{4}$ 0 7	$\bar{4}$ 10 0	1.8206	11.58	1.827	12
4 0 3	4 8 0	1.8094	9.33		
1 3 4	1 9 3	1.7893	4.12	1.789	8
$\bar{8}$ 0 7		1.7881	2.18		
$\bar{6}$ 4 4	$\bar{6}$ 2 4	1.7435	8.44	1.751	12
$\bar{6}$ 4 2	$\bar{6}$ $\bar{2}$ 4	1.7406	7.04		
$\bar{3}$ 5 2	$\bar{3}$ 3 5	1.7280	3.65		
7 3 6	$\bar{7}$ 5 3	1.7113	3.08		
$\bar{4}$ 2 7	$\bar{4}$ 10 2	1.6907	7.36	1.695	21
0 4 4	0 8 4	1.6888	24.94		
4 2 3	4 10 2	1.6818	6.11		
3 5 0	3 3 5	1.6779	8.03		
$\bar{8}$ 2 7	$\bar{8}$ 6 2	1.6646	9.54	1.660	14
$\bar{8}$ 2 1	$\bar{8}$ 6 2	1.6544	9.02		
$\bar{6}$ 0 8	$\bar{6}$ 10 0	1.6409	3.31		
$\bar{8}$ 0 8	$\bar{8}$ 8 0	1.6197	7.31	1.622	11
8 0 0	8 8 0	1.6072	7.45		
$\bar{3}$ 5 4	$\bar{3}$ 5 5	1.5939	7.16	1.583	9
$\overline{10}$ 2 5	$\overline{10}$ 0 2	1.5775	0.08		
7 3 0	7 7 3	1.5720	3.33		
$\bar{6}$ 4 6	$\bar{6}$ 6 4	1.5677	3.32		
4 4 2	4 8 4	1.5644	2.33	1.565	12
6 4 0		1.5612	1.33		
$\overline{10}$ 2 6	$\overline{10}$ 2 2	1.5612	4.50		
$\overline{10}$ 2 4	$\overline{10}$ $\bar{2}$ 2	1.5577	2.79	1.550	13

* Experimental data on radtkeite taken from McCormack *et al.* (1991). Values of *d* are quoted in Å.

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