Iwashiroite-(Y), YTaO₄, a new mineral from Suishoyama, Kawamata Town, Fukushima Prefecture, Japan

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Iwashiroite-(Y), YTaO₄, was found from Suishoyama, Kawamata Town, Fukushima Prefecture, Japan. It is monoclinic, $P2_1/a$, $a = 5.262(5)$ Å, $b = 5.451(5)$ Å, $c = 5.110(5)$ Å, $\beta = 95.12(10)^\circ$, $V = 146.0(2)$ Å³, $Z = 2$. The five strongest lines in the powder XRD pattern [$d(\text{Å})$, I/I_0 , hkl] are (3.13, 100, $\bar{1}11$), (2.95, 94, 111), (2.73, 26, 020), (1.890, 29, 220) and (1.862, 29, 022). Electron microprobe analysis gave; Y₂O₃ 29.10, Ce₂O₃ 0.10, Nd₂O₃ 0.10, Sm₂O₃ 0.36, Gd₂O₃ 1.06, Tb₂O₃ 0.25, Dy₂O₃ 2.38, Ho₂O₃ 0.56, Er₂O₃ 2.09, Tm₂O₃ 0.37, Yb₂O₃ 3.33, Lu₂O₃ 0.85, ThO₂ 0.02, UO₂ 0.15, CaO 0.17, Ta₂O₅ 40.64, Nb₂O₅ 16.66, TiO₂ 0.41, total 98.60 wt%, and leads to the empirical formula, (Y_{0.81}Yb_{0.05}Dy_{0.04}Er_{0.03}Gd_{0.02}Lu_{0.01}Ho_{0.01}Sm_{0.01}Ca_{0.01}Tm_{0.01})_{Σ1.00}(Ta_{0.58}Nb_{0.39}Ti_{0.02})_{Σ0.99}O₄ on the basis of the 4 oxygen atoms per formula unit. Iwashiroite-(Y) is translucent and amber brown to brown in color with a glassy to subadamantine luster. The streak is pale brown and cleavage is {010} good, {001} poor. The Mohs' hardness is 6. The calculated density is 7.1 g/cm³. Iwashiroite-(Y) occurs as an aggregate of small euhedral platy crystals with a metamict substance in the main ore body of the granite pegmatite mine at the locality. Associated minerals are quartz, microcline and annite. The crystal structure was refined to $R = 0.034$ with single crystal XRD data. Although the structure consists of TaO₆ octahedra and YO₈ polyhedra, iwashiroite-(Y) is not isostructural with fergusonite-beta-(Y).

Keywords: Iwashiroite, New mineral, Yttrium, Tantalum, Suishoyama

INTRODUCTION

Suishoyama is well known in Japan as an area rich in minerals containing rare metals, such as yttrium, lanthanides, niobium, tantalum, zirconium, uranium and lithium. More than 20 species of rare metal minerals have been reported in this locality. During a survey of the main ore body of the granite pegmatite mine, one of the authors of this paper (TK) found an amber brown aggregate around 7 mm in size. Preliminary XRF analysis revealed that this mineral contained a considerable amount of yttrium and tantalum as its main constituents. The chemical composition suggests a close relationship to forman-

ite-(Y) (Kornetova and Kazakova, 1964) and yttrotantalite (Vlasov, 1964). These minerals occur in the metamict state, and consequently, their descriptions are inadequate. The present yttrium tantalate mineral from Suishoyama gave sharp diffraction peaks in the preliminary XRD investigation with a conventional powder X-ray diffractometer. The XRD pattern is not identical with those of annealed samples of metamict formanite-(Y) (Kornetova and Kazakova, 1964) and yttrotantalite-(Y) (Anthony et al., 1997).

This yttrium tantalate mineral was named as iwashiroite-(Y) after the old province name of the locality, Iwashiro, the central part of Fukushima Prefecture, and in accordance with the Levinson rule. The mineral data and the name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association (#2003-053). The type specimen is deposited at the National Science Museum, Tokyo, under the registered number NSM-M28537.

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OCCURRENCE

Iwashiroite was found in the pegmatite deposits of the Suishoyama mine, Kawamata Town, Fukushima Prefecture, Japan. The mine is situated in the NW part of Abukuma belt, where is characterized by regional metamorphic rocks and granitic rocks containing many pegmatites. The pegmatites around the Suishoyama mine range north and south over a distance of about 2 km (Ohara et al., 2000). The Suishoyama No.1 Pit is the largest pegmatite body in this area (140°37'E, 37°40'N). The modern mining activity began in 1916, and in the 1950s the mine produced about 150 tons of quartz and 100 tons of feldspars per month. However, the operation closed in the early 1980s.

After the first mineralogical research by Mr. Otokichi Nagashima in 1937, rare earth element (REE)-minerals have attracted the attentions of many investigators. For example, tenerite-(Y) (Iimori, 1938), 'abukumalite' (Hata, 1938) and allanite-(Ce) (Hata, 1939) were reported with the old locality name of Iizaka or Iisaka Village. Among them, 'abukumalite' was proposed as a new mineral, but it is now known to correspond to britholite-(Y). Tenerite-(Y) was redefined as Y₂(CO₃)₃·nH₂O with the establishment of two neo-type specimens from Ytterby and Suishoyama (Miyawaki et al., 1993). In addition, other REE-minerals have been found, such as thalenite-(Y) (Kato, 1973), yttrialite-(Y) (Omori and Hasegawa, 1953), a new mineral, iimoriite-(Y) (Kato and Nagashima, 1970) and caysichite-(Y) (Yamada et al., 2004). A new amphibole, protomangano-ferro-anthophyllite, was described in fayalite, one of the constituents of the pegmatite (Sueno et al., 1998, 2002).

The specimen including iwashiroite-(Y) was collected at a dump near the No. 1 Pit. The mixture of crystalline iwashiroite-(Y) and a metamict substance with a similar chemical composition occurred as an aggregate of small euhedral platy crystals up to 7 mm in width (Fig. 1). The associated minerals are quartz, microcline and annite. The specimen shows zoning, which appeared as contrast on a back scattered electron image (Fig. 2). The contrast depends on the U contents. The darker parts, iwashiroite-(Y), with less U give X-ray diffraction, whereas brighter parts give no X-ray diffraction. The crystal form is almost square plate. The prominent crystal face is (010). Striation in the [101] direction is observed on (010) face frequently. The angle between striation and (001) is 44.15°.

PHYSICAL AND OPTICAL PROPERTIES

Iwashiroite-(Y) is amber brown to brown in color with a pale brown streak. It is translucent with a glassy to sub-

Table 1. Reflectance values for iwashiroite-(Y)

	Air		Oil	
	Max	Min	Max	Min
400 nm	15.3	14.4	5.2	5.2
420 nm	14.9	14.3	4.6	4.4
440 nm	14.4	14.0	4.4	4.2
460 nm	14.2	13.9	4.3	4.1
470 nm	14.1	13.8	4.4	4.1
480 nm	14.0	13.7	4.4	4.1
500 nm	13.9	13.7	4.4	4.1
520 nm	13.8	13.5	4.4	4.0
540 nm	13.8	13.5	4.5	4.0
546 nm	13.8	13.6	4.5	4.0
560 nm	13.8	13.6	4.6	4.1
580 nm	13.9	13.6	4.7	4.1
589 nm	13.9	13.6	4.8	4.2
600 nm	13.9	13.7	4.8	4.3
620 nm	14.0	13.8	5.0	4.5
640 nm	14.0	13.8	5.1	4.6
650 nm	14.0	13.7	5.0	4.6
660 nm	14.0	13.8	5.1	4.7
680 nm	14.1	13.9	5.3	5.0
700 nm	14.3	14.1	5.9	5.8

Values recommended by the Commission on Ore Mineralogy of International Mineralogical Association are given in bold face.

adamantine luster (Fig. 1). Cleavage is good on {010} and poor on {001}. The calculated density is 7.1 g/cm³. Vickers microhardness is 766–825 kg/cm² (50 g load), corresponding to 6 on the Mohs' scale. Fracture is sub-conchoidal, and tenacity is brittle. Refractive indices could not be measured due to the very small dimensions of the crystals and to the association with the metamict substance. Reflectance spectra in air and in oil (Nikon nD = 1.515) for iwashiroite-(Y) were measured relative to a SiC standard (Zeiss No.851) (Table 1). No fluorescence was observed under ultraviolet radiation of 254 and 365 nm.

CHEMICAL COMPOSITION

Preliminary XRF analysis indicated that the mineral consisted of Y, Ln (lanthanides), Ta, and Nb. A further analysis with an EDS electron microprobe analyzer revealed that it contains small amounts of Ti, Th, U and Ca, in addition to the major elements. No other elements with atomic numbers greater than ten were detected. A quantitative analysis was carried out with a JEOL JXA-8800M WDS electron microprobe analyzer (accelerating voltage, 15 kV; beam current, 10 nA; beam size, 2 μm) for 18 analytical spots (Table 2). Standard deviations are given in parentheses following the averages.

The empirical formulae on the basis of the 4 oxygen atoms per formula unit are: (Y_{0.81}Yb_{0.05}Dy_{0.04}Er_{0.03}Gd_{0.02}

Table 2. Chemical composition for iwashiroite-(Y)

Constituent	Crystalline part		Metamict part	Standard
	Average (wt%)	Range (wt%)	Average (wt%)	
Y ₂ O ₃	29.10(41)	28.43-29.77	24.63	YP ₅ O ₁₄
La ₂ O ₃	n.d.			LaP ₅ O ₁₄
Ce ₂ O ₃	0.10(10)	0.00-0.26	0.11	CeP ₅ O ₁₄
Pr ₂ O ₃	n.d.			PrP ₅ O ₁₄
Nd ₂ O ₃	0.10(5)	0.04-0.19	0.46	NdP ₅ O ₁₄
Sm ₂ O ₃	0.36(10)	0.27-0.61	0.72	SmP ₅ O ₁₄
Eu ₂ O ₃	n.d.			EuP ₅ O ₁₄
Gd ₂ O ₃	1.06(19)	0.69-1.30	1.41	GdP ₅ O ₁₄
Tb ₂ O ₃	0.25(14)	0.00-0.49	0.38	TbP ₅ O ₁₄
Dy ₂ O ₃	2.38(16)	2.08-2.65	3.17	DyP ₅ O ₁₄
Ho ₂ O ₃	0.56(12)	0.41-0.81	0.64	HoP ₅ O ₁₄
Er ₂ O ₃	2.09(12)	1.85-2.28	2.5	ErP ₅ O ₁₄
Tm ₂ O ₃	0.37(18)	0.11-0.68	0.63	TmP ₅ O ₁₄
Yb ₂ O ₃	3.33(17)	3.07-3.62	4.09	YbP ₅ O ₁₄
Lu ₂ O ₃	0.85(21)	0.48-1.15	1.11	LuP ₅ O ₁₄
ThO ₂	0.02(3)	0.00-0.09	0.29	ThO ₂
UO ₂	0.15(10)	0.03-0.32	1.87	UO ₂
CaO	0.17(2)	0.14-0.22	0.12	Wollastonite
Ta ₂ O ₅	40.64(72)	39.28-42.03	38.93	Tantalite
Nb ₂ O ₅	16.66(45)	16.13-17.54	15.77	Ferrocolumbite
TiO ₂	0.41(15)	0.15-0.66	0.73	Anatase
Total	98.6		97.56	

n.d., not detected.

Lu_{0.01}Ho_{0.01}Sm_{0.01}Ca_{0.01}Tm_{0.01})_{Σ1.00}(Ta_{0.58}Nb_{0.39}Ti_{0.02})_{Σ0.99}O₄ for the crystalline part, and (Y_{0.71}Yb_{0.07}Dy_{0.06}Er_{0.04}Gd_{0.03}U_{0.02}Lu_{0.02}Sm_{0.01}Ho_{0.01}Tm_{0.01}Nd_{0.01}Ca_{0.01}Tb_{0.01})_{Σ1.01}(Ta_{0.58}Nb_{0.39}Ti_{0.03})_{Σ1.00}O₄ for the metamict part. The simplified formula is Y(Ta,Nb)O₄, and the ideal formula is YTaO₄, which requires Y₂O₃ 33.82, Ta₂O₅ 66.18 (wt%).

CRYSTALLOGRAPHY AND CRYSTAL STRUCTURE

The X-ray powder diffraction pattern for iwashiroite-(Y) was obtained using a Gandolfi camera with diameter = 114.6 mm employing Ni-filtered CuK α radiation. The data were recorded on an imaging plate, and processed with a Fuji BAS-2500 bio-image analyzer using computer program written by Nakamuta (1999). The powder X-ray diffraction data of iwashiroite-(Y) are given in Table 3, with those of synthetic YTaO₄ for comparison. Iwashiroite-(Y) is monoclinic with space group of *P2₁/a*. The unit cell parameters were refined from the powder X-ray diffraction data with an internal SiO₂-standard reference material (NIST 1878a) using a computer program by Toraya (1993); *a* = 5.262(5) Å, *b* = 5.451(5) Å, *c* =

5.110(5) Å, β = 95.12(10)°, *V* = 146.0(2) Å³, and *Z* = 2.

The X-ray diffraction intensity data of a single crystal for structure analysis were collected using a Rigaku RASA-7R four-circle diffractometer employing graphite monochromatized MoK α radiation (56 kV, 270 mA). Experimental details of the data collection are given in Table 4. The length of *b*-axis of iwashiroite-(Y) is approximately half of that of fergusonite-beta-(Y), although the lengths of *a*- and *c*-axes and angle of β of iwashiroite-(Y) are comparable to those of fergusonite-beta-(Y). No diffraction peaks arising from double the *b*-axis length were observed in the collected intensity data from the pseudo-double lattice of iwashiroite-(Y). Data reduction to *Fo*² with Lorentz and polarization corrections and correction for absorption (φ -scan procedure) were carried out with a computer program by Dr. Kazumasa Sugiyama of the University of Tokyo (personal communication). The SHELXL-97 software package (Sheldrick, 1997) was employed to refine the crystal structure. The scattering factors for the neutral atoms and anomalous dispersion factors were taken from the International Tables for X-ray Crystallography, Volume C (1992). Full matrix least-squares refinement was performed by refining the

Table 3. Powder X-ray diffraction data obtained with a Gandolfi camera and Imaging Plate*

<i>h</i>	<i>k</i>	<i>l</i>	Present study			YTaO ₄ **		<i>h</i>	<i>k</i>	<i>l</i>	Present study			YTaO ₄ **	
			<i>I</i>	<i>d</i> _{obs.}	<i>d</i> _{calc.}	<i>I</i>	<i>d</i> _{obs.}				<i>I</i>	<i>d</i> _{obs.}	<i>d</i> _{calc.}	<i>I</i>	<i>d</i> _{obs.}
0	1	0	4	5.46	5.45	5	5.44	$\bar{2}$	2	2	10	1.566	1.566	10	1.579
0	0	1	3	5.08	5.09	8	5.07	3	1	1	12 [†]	1.544	1.543	12	1.5378
1	1	0			3.78	14	3.78	$\bar{1}$	1	3	4	1.515	1.512	14	1.5001
0	1	1	8	3.72	3.72	10	3.72	$\bar{2}$	3	0	3	1.494	1.493		
$\bar{1}$	1	1	100	3.13	3.13	100	3.161	0	3	2	10	1.473	1.479	8	1.4756
1	1	1	94	2.95	2.94	85	2.920	2	2	2			1.472		
0	2	0	26	2.73	2.73	20	2.723	3	2	0			1.471		
2	0	0	23	2.62	2.62	25	2.629	$\bar{2}$	3	1			1.453	12	1.4597
0	0	2	2	2.56	2.54	18	2.536	$\bar{3}$	2	1			1.442	3	1.4527
$\bar{2}$	0	1			2.42	6	2.449	$\bar{2}$	1	3			1.434	3	1.4476
1	2	0	8	2.42	2.42	12	2.419	$\bar{1}$	2	3			1.416	4	1.4212
0	2	1			2.40	3	2.399	2	3	1	6	1.414	1.413	6	1.4088
2	1	0			2.36	2	2.368	3	2	1			1.385	1	1.3809
0	1	2			2.31	3	2.300	2	0	3			1.369		
$\bar{2}$	1	1			2.21	3	2.232	0	4	0	4	1.362	1.363		
$\bar{1}$	1	2			2.18	2	2.191	1	2	3			1.363		
1	2	1	10	2.15	2.15	14	2.141	1	4	0	11	1.319	1.319		
2	1	1	4	2.08	2.08	5	2.067	$\bar{2}$	3	2			1.317		
1	1	2			2.05	2	2.033	$\bar{3}$	2	2			1.317		
$\bar{2}$	0	2	19	1.914	1.913	20	1.938	$\bar{3}$	1	3	0		1.242		
2	2	0	29	1.890	1.889	25	1.892	$\bar{3}$	3	1	8	1.242	1.241		
0	2	2	29	1.862	1.860	30	1.856	0	3	3			1.240		
$\bar{2}$	1	2	2 [†]	1.822	1.805	4	1.824	$\bar{1}$	3	3	4	1.224	1.225		
0	3	0			1.817	4	1.815	3	3	1	9	1.203	1.205		
$\bar{1}$	2	2	5	1.792	1.790	8	1.798	0	4	2			1.201		
2	0	2	13	1.752	1.749	16	1.732	1	3	3			1.189		
1	2	2	14	1.713	1.718	16	1.708	$\bar{2}$	0	4	5	1.190	1.187		
1	3	0			1.717			4	2	0			1.181		
0	3	1			1.711			$\bar{1}$	4	2	5 [†]	1.184	1.182		
0	0	3			1.696	2	1.692	1	4	2	2	1.159	1.160		
2	1	2			1.666	4	1.650	$\bar{3}$	2	3			1.155		
3	1	0			1.664	2	1.667	0	2	4			1.153		
$\bar{1}$	3	1	18	1.642	1.641	16	1.644	$\bar{2}$	3	3	3	1.152	1.150		
$\bar{3}$	1	1	18	1.623	1.623	25	1.637	3	1	3	2	1.140	1.140		
0	1	3			1.620	4	1.616	4	0	2	2	1.126	1.125		
1	3	1	20	1.614	1.612	8	1.608	2	0	4	4	1.108	1.106		
$\bar{1}$	1	3	9	1.587	1.586	16	1.593	$\bar{4}$	2	2			1.106		

$$a = 5.262(5) \text{ \AA}, b = 5.451(5) \text{ \AA}, c = 5.110(5) \text{ \AA}, \beta = 95.12(10)^\circ, V = 146.0(2) \text{ \AA}^3$$

* The data were calibrated with internal SiO₂-standard reference material (NIST 1878a).

** Synthetic YTaO₄, ICDD#24-1425.

[†] Estimated from data with the external standard reference material, because of overlap by the diffraction of SiO₂-standard.

positional parameters, scale factor, and displacement parameters. The atomic positional parameters of synthetic YTaO₄ (Wolten, 1964) were used as the initial parameters in the present refinement. The site occupancy factors (*sof*) were fixed according to the chemical composition. The final positional parameters and anisotropic displacement parameters with equivalent isotropic displacement parameters are given in Table 5. Selected interatomic distances are summarized in Table 6. The bond valences were calculated from the interatomic distances following the procedure of Brown and Altermatt (1985) using the parameters of Brese and O'Keeffe (1991). The values listed in Table 6 are weighted averages according to the occupan-

cies in the final refinement (Table 5).

DISCUSSION

Iwashiroite-(Y) is isostructural with a synthetic yttrium tantalate, YTaO₄ (Wolten, 1967). The tantalum atom in iwashiroite-(Y) is coordinated by 4 and additional 2 oxygen atoms (Table 6). The values of bond valence sum for the tantalum atom in iwashiroite-(Y) are 4.06 and 4.92 for tetragonal and octahedral coordinations, respectively. The latter value is much closer to the ideal valency of Ta, 5, and suggests that the coordination polyhedron of Ta should be a distorted octahedron rather than a tetrahedron.

Table 4. Crystallographic data and experimental details

a (Å)	5.292(2)
b (Å)	5.452(2)
c (Å)	5.1149(18)
β (°)	95.89(3)
V (Å ³)	146.80(10)
Space group	$P2_1/a$
Z	2
Formula	$\text{Y}_{0.78}\text{Ln}_{0.22}\text{Ta}_{0.60}\text{Nb}_{0.40}\text{O}_4$
D_{calc} (g/cm ³)	7.135
μ (cm ⁻¹)	44.9
Crystal dimension (mm)	0.03 x 0.03 x 0.01
Diffractometer	Rigaku AFC-7R
Radiation	MoK α (graphite)
Scan mode, rate (°/min in ω)	2θ - ω , 8
2θ range	5–65
Reflection range	$-6 \leq h \leq 3$ $-7 \leq k \leq 0$ $-6 \leq l \leq 6$
No. of measured reflections	583
No. unique reflections	493
No. of observed reflections [$I > 2\sigma(I)$]	429
R_{int}	0.0360
Variable parameters	29
$R1$ [$I > 2\sigma(I)$], $R1$ (all reflections)	0.0340, 0.0439
$wR2$ (all reflections)	0.1062
Weighting parameters, a , b	0.1, 0
Goodness of Fit	0.848
Final $\Delta\rho_{\text{min}}$ (e/Å ³)	-2.373
Final $\Delta\rho_{\text{max}}$ (e/Å ³)	3.339

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

$$wR2 = \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]^{0.5}$$

$$w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$$

$$P = [2F_c^2 + F_o^2] / 3$$

Table 5. Final atomic coordinates and displacement parameters (Å²)*

	x	y	z	U_{eq}		
Y	0.25	0.76342(17)	0	0.0076(2)		
Ta	0.25	0.30254(11)	0.5	0.0088(2)		
O1	0.4922(10)	0.4360(12)	0.2669(10)	0.0096(11)		
O2	0.0975(11)	0.0868(11)	0.2514(11)	0.0111(11)		
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y	0.0065(5)	0.0056(4)	0.0110(4)	0	0.0019(3)	0
Ta	0.0077(4)	0.0069(3)	0.0118(3)	0	0.00108(19)	0
O1	0.010(3)	0.007(2)	0.012(3)	-0.0056(19)	0.003(2)	-0.002(2)
O2	0.010(3)	0.009(3)	0.015(3)	-0.0023(19)	-0.0004(19)	0.002(2)

* Occupancy: Y: 0.78Y + 0.22Ho; Ta: 0.60Ta + 0.40Nb

Table 6. Interatomic distances (Å) and bond valences

Y–O2	2.284(6)	x2	0.49 x2	Ta–O2	1.855(6)	x2	1.18 x2
–O1	2.300(5)	x2	0.47 x2	–O1	1.977(5)	x2	0.85 x2
–O2	2.372(6)	x2	0.39 x2	–O1	2.232(6)	x2	0.43 x2
–O1	2.517(6)	x2	0.26 x2				
				<Ta–O> ₄	1.916		4.06
<Y–O> ₈	2.368		3.22	<Ta–O> ₆	2.021		4.92

Figure 1. A photomicrograph of an aggregate of minute crystals of iwashiroite-(Y). Some of the aggregates appear dark blue owing to internal reflections.

Figure 2. A back scattered electron image of a fragment of iwashiroite-(Y). The dark parts are U-poor and give X-ray diffraction. The present data were obtained from the crystalline part.

Table 7. Crystallographic data for iwashiroite-(Y), formanite-(Y), fergusonite-beta-(Y) and fergusonite-(Y)

Iwashiroite-(Y)	Formanite-(Y)	Fergusonite-beta-(Y)*	Fergusonite-(Y)
YTaO ₄	YTaO ₄	YNbO ₄	YNbO ₄
Monoclinic	Tetragonal	Monoclinic	Tetragonal
<i>P</i> 2/ <i>a</i>	<i>P</i> 4/ <i>m</i> , <i>P</i> 4 ₂ / <i>m</i> , <i>P</i> 4/ <i>n</i> or <i>P</i> 4 ₂ / <i>n</i>	<i>I</i> 2/ <i>a</i>	<i>I</i> 4 ₁ / <i>a</i>
<i>a</i> = 5.292(2) Å	<i>a</i> = 7.75 Å	<i>a</i> = 5.243 Å	<i>a</i> = 5.16 Å
<i>b</i> = 5.452(2) Å		<i>b</i> = 10.841 Å	
<i>c</i> = 5.1149(18) Å	<i>c</i> = 11.41 Å	<i>c</i> = 5.046 Å	<i>c</i> = 10.89 Å
β = 95.89(3)°		β = 94.50°	
<i>V</i> = 146.80(10) Å ³	<i>V</i> = 685 Å ³	<i>V</i> = 285.9 Å ³	<i>V</i> = 290 Å ³
<i>Z</i> = 2	<i>Z</i> = ?	<i>Z</i> = 4	<i>Z</i> = 4
Present study	Palache et al. (1944)	Kinzhbalo et al. (1982)	Komkov (1959)

* Data for synthetic YbNbO₄.

Figure 3. A comparison of the crystal structures and crystallographic data of iwashiroite-(Y), formanite-(Y), fergusonite-beta-(Y) and fergusonite-(Y). The TaO₆ and NbO₆ octahedra in iwashiroite-(Y) and fergusonite-beta-(Y) are shown in brown. The coordination polyhedra of Nb in fergusonite-(Y) are illustrated as brown NbO₈ polyhedra, instead of NbO₄ tetrahedra. All the Y atoms in the structures are denoted by yellow spheres.

The Ta-octahedra share their edges to form zigzag chains running parallel to the *c*-axis (Fig. 3). The yttrium atom in iwashiroite-(Y) is coordinated with 8 oxygen atoms to form a YO₈ distorted cube. The Ta-zigzag chains are connected by the Y atoms.

Iwashiroite-(Y) is not isostructural with fergusonite-beta-(Y) (Table 7 and Fig. 3). However, these minerals consist of very similar structural components, the zigzag chains of Ta- or Nb-octahedra with 8-coordinated Y atoms. Figure 3 shows the differences in the configuration of the components in their respective crystal structures. These similarities and differences are reflected in the lattice parameters, as described above. The distinctive characteristic of the crystal structure of iwashiroite-(Y) is the alternating arrangement of the Y- and Ta-walls perpendicular to the *a*-axis.

The mean Y-O interatomic distance in iwashiroite-(Y) is 2.368 Å, and is comparable to the mean Y-O interatomic distance in synthetic YTaO₄, 2.35 Å (Wolten, 1967). As indicated in the empirical formula, the Y site in iwashiroite-(Y) is predominantly occupied by yttrium with a small amount of lanthanides having ionic radii similar to yttrium. The replacement of yttrium with such lanthanides at the Y site of iwashiroite-(Y) is reasonable due to the similar interatomic distances to the Y-O distances in synthetic YTaO₄. In contrast, approximately 40% of the tantalum is substituted with niobium at the Ta site of iwashiroite-(Y). This substitution apparently shortens the mean distance for the four shortest Ta-O interatomic distances of 1.916 Å compared with the mean distance for synthetic YTaO₄ of 1.99 Å. However, it is worth noting that the substitution of the smaller Nb ion for the larger Ta ion does not simply affect the two longest Ta-O bond distances. The distance in iwashiroite-(Y), 2.232 Å, is longer than that in synthetic YTaO₄, 2.14 Å, in spite of the introduction of the smaller Nb ion at the Ta site.

The lack of crystallographic data for formanite-(Y) and yttrotantalite-(Y), which occur in the metamict state, has been a problem in the understanding of rare earth tantalate minerals. Iwashiroite-(Y), the third natural phase of rare earth tantalate, is a monoclinic phase with formanite-(Y) composition. Chemically, it is a Ta-analogue of fergusonite-(Y) and fergusonite-beta-(Y). However, it is not isomorphous with fergusonite-beta-(Y) (Fig. 3), but is a natural analogue of synthetic YTaO₄ (Wolten, 1967). Wolten (1967) described synthetic YTaO₄ as an *M'*-phase having a different crystal structure from the *M*-phase, i.e., monoclinic fergusonite-beta-(Y). The relationship between iwashiroite-(Y) and formanite-(Y) is not clear, because the crystal structure of formanite-(Y) has not been clarified (Fig. 3). Iwashiroite-(Y) is not a simple Ta-analogue of fergusonite-beta-(Y), whereas it shows a

solid solution towards YNbO₄, the ideal compositions of fergusonite-beta-(Y) and fergusonite-(Y). Therefore, the relationship between fergusonite-beta-(Y) and fergusonite-(Y) (Fig. 3) is not applicable to the relationship between iwashiroite-(Y) and formanite-(Y). This is the reason why this new mineral was not named as "formanite-beta-(Y)".

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