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$BaY_{16}Si_4O_{33}$ containing $Ba(SiO_4)_4$ orthosilicates

Shuto Motozawa,[a,b] Hiromitsu Kimura,[c] Junichi Takahashi,[a] Rayko Simura[a] and Hisanori Yamane[a]*

[a]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Katahira 2-1-1 Aoba-ku, Sendai 980-8577, Japan, [b]Department of Metallurgy, Materials Science and Materials Processing, Graduate School of Engineering, Tohoku University, 6-6-4 Aramaki Aza Aoba, Aoba-ku, Sendai 980-8579, Japan, and [c]Science & Innovation Center, Inorganic Materials Laboratory, Mitsubishi Chemical Corporation, 1000 Kamoshida-cho, Aoba-ku, Yokohama 227-8502, Japan. *Correspondence e-mail: hisanori.yamane.a1@tohoku.ac.jp

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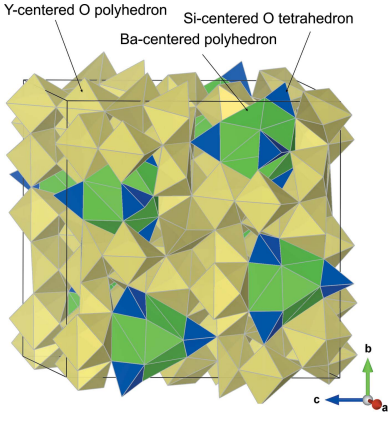
Single crystals of a new quaternary oxide, barium hexadecayttrium tetrasilicon tritriacontaoxide, $BaY_{16}Si_4O_{33}$, were obtained from a melt-solidified sample prepared by heating a mixture of $BaCO_3$, Y_2O_3, and SiO_2 at 2073 K. X-ray crystal structure analysis revealed that $Ba(SiO_4)_4$ orthosilicate clusters in which a Ba atom is surrounded by four SiO_4 tetrahedra were isolated in a framework composed of Y and O in the structure of $BaY_{16}Si_4O_{33}$. The dielectric constant measured for polycrystalline ceramics of $BaY_{16}Si_4O_{33}$ sintered at 1953 K was 13 (298 K, 1 MHz), and the thermal expansion coefficient was 8.70×10^{-6} K^{-1} (298–873 K), which are close to the values previously reported for Y_2O_3.

1. Chemical context

Numerous silicates in minerals and ceramic materials have been studied (Liebau, 1985). Silicates have also attracted attention as host materials for phosphors because of their structural diversity and stability (Gupta *et al.*, 2021, Singh *et al.*, 2017). In the Ba–Y–Si–O system, $BaY_2Si_3O_{10}$, $Ba_9Y_2Si_6O_{24}$, $BaY_4Si_5O_{17}$, $Ba_{5.2}Y_{13}Si_8O_{41}$, and $Ba_2Y_2Si_4O_{13}$ have been reported. Among these oxides, phosphors based on Pr^{3+}, Sm^{3+}, Er^{3+}, Ce^{3+}, Tb^{3+}, and Eu^{3+} doping of $BaY_2Si_3O_{10}$ (Wierzbicka-Wieczorek *et al.*, 2015; Xia *et al.*, 2014; Zhou & Xia, 2015; Liu *et al.*, 2009), Pr^{3+}, Sm^{3+}, Er^{3+}, and Ho^{3+} doping of $BaY_4Si_5O_{17}$ (Wierzbicka-Wieczorek *et al.*, 2015), Ce^{3+} doping of $Ba_9Y_2Si_6O_{24}$ (Liu *et al.*, 2015; Brgoch *et al.*, 2013), and Bi^{3+} and Eu^{3+} doping of $Ba_2Y_2Si_4O_{13}$ (Song *et al.*, 2019) as activator ions have been studied. Recently, $BaY_2Si_3O_{10}$ has been investigated for its potential application as a microwave dielectric material for 5G communication devices (Lin *et al.*, 2020). In the present study, we found a new quaternary oxide, $BaY_{16}Si_4O_{33}$, with a Y_2O_3 content greater than that of previously reported compounds in the Ba–Y–Si–O system.

The dielectric constants measured at 100 Hz and 1 MHz for $BaY_{16}Si_4O_{33}$ ceramics at 298 K were 14 and 13, respectively, and the dielectric loss was less than 0.01 (Figs. S1 and S2). These dielectric constants are close to the value reported for Y_2O_3 ceramics (12; Tsukuda, 1980) and the values measured for Y_2O_3 fabricated by oxidation of Y metal on Si substrates (17–20; Manchanda & Gurvitch, 1988). The temperature coefficient of the dielectric constant at 298–413 K was 3.5×10^{-3} K^{-1}. The thermal expansion coefficient measured for the polycrystalline $BaY_{16}Si_4O_{33}$ in the temperature range 298–873 K was 8.7×10^{-6} K^{-1} (Fig. S3). This value is in good agreement with the thermal expansion coefficient of Y_2O_3 of



8.5×10^{-6} K^{-1} in the temperature range 298–1272 K (Kirchner, 1964). In $BaY_{16}Si_4O_{33}$, the portion of Y–O frameworks in the crystal structure is large, which might be related to the fact that the dielectric constant and thermal expansion coefficient of $BaY_{16}Si_4O_{33}$ and Y_2O_3 are similar to each other.

2. Structural commentary

The literature contains no reports of silicates or other oxides with the same structure as $BaY_{16}Si_4O_{33}$. In the crystal structure of $BaY_{16}Si_4O_{33}$, clusters composed of a Ba atom surrounded by four isolated SiO_4 tetrahedra are isolated in a three-dimensional framework formed by 16 Y sites with six- or sevenfold coordination to oxygen atoms within an interatomic distance of 2.65 Å (Figs. 1 and 2). $BaY_{16}Si_4O_{33}$ has a large portion of Y in the cation sites, and more than one-half of the oxygen atoms are not bonded to Si. Thus, $BaY_{16}Si_4O_{33}$ can be expressed as an oxide silicate with the formula $Y_{16}O_{17}Ba(SiO_4)_4$.

The Si—O bond lengths for the SiO_4 tetrahedra range from 1.6198 (17) to 1.6596 (18) Å (Table 1). Bond-valence sums (BVSs) of 3.85 to 4.01, which are similar to the Si formal valence of IV, were calculated using the bond-valence parameter of Gagné & Hawthorne (2015). Ba1 is coordinated by twelve oxygen atoms of four SiO_4 tetrahedra with Ba1—O distances ranging from 2.7478 (18) to 3.274 (2) Å. The BVS for Ba1 is 2.10, which is close to the formal Ba valence of II.

The respective average distances between the sixfold-coordinated Y1–6, Y8–10, and Y12 sites and oxygen are between 2.275 and 2.308 Å, which are approximately equal to the Y1—O1 distance [2.2847 (11) Å] and Y2—O1 average distance (2.282 Å) for sixfold Y coordination reported for Y_2O_3 (Coduri *et al.*, 2013). The respective average distances between oxygen atoms and sevenfold-coordinated Y7, Y11, Y13, and Y14–16 are 2.342–2.366 Å, which are close to the Y2—O average distance of 2.360 Å reported for sevenfold-coordinated Y in the structure of Y_2SiO_5 (Denault *et al.*, 2015). The BVSs ranged from 2.77 to 2.97, close to the Y valence of III.

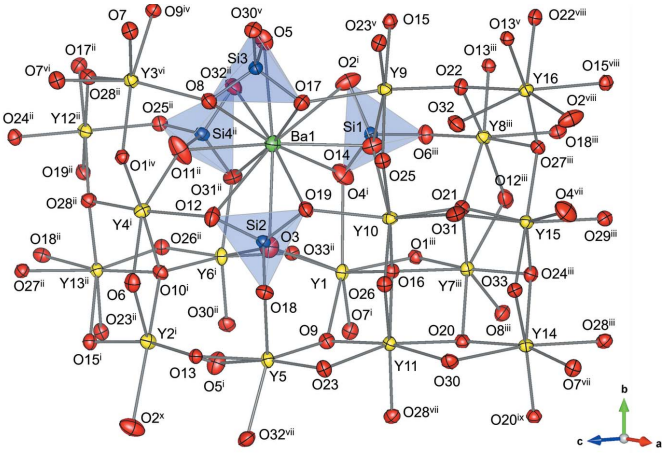


Figure 1
The atomic arrangement of $BaY_{16}Si_4O_{33}$ depicted with displacement ellipsoids at the 80% probability level. [Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $-x, -y+1, -z+1$; (vii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (viii) $-x+1, -y+1, -z$; (ix) $-x+1, -y, -z$; (x) $x, y-1, z$.]

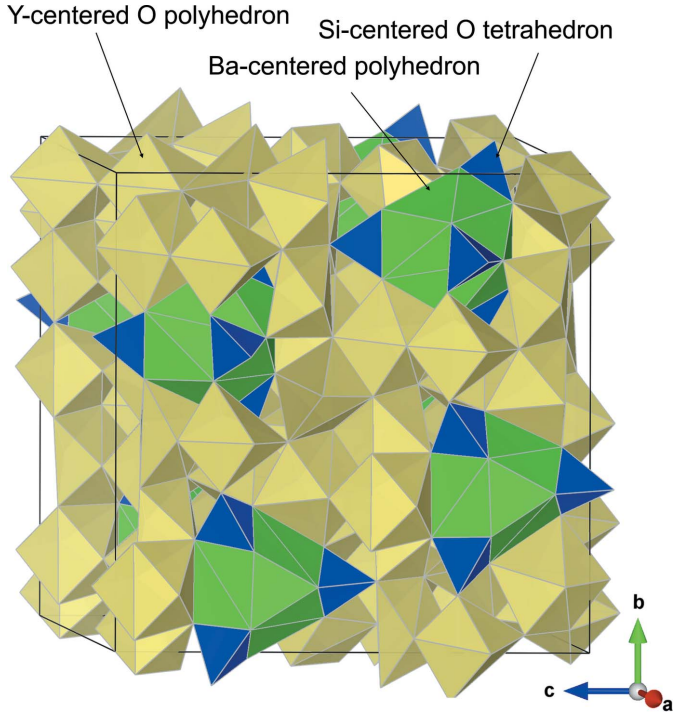


Figure 2
A polyhedral representation of $BaY_{16}Si_4O_{33}$ showing the Y-centered oxygen polyhedra (yellow) and the Ba-centered oxygen polyhedra (green) surrounded by isolated Si-centered oxygen tetrahedra (blue).

The Madelung part of the lattice energy (MAPLE; Hoppe, 1970) for $BaY_{16}Si_4O_{33}$, as calculated using the *VESTA* software (Momma & Izumi, 2011), is −186,000 kJ mol^{-1}. The difference between the MAPLE for $BaY_{16}Si_4O_{33}$ and the sum of the MAPLEs (−186,999 kJ·mol^{-1}) for binary oxides with the formula $BaY_{16}Si_4O_{33}$ (= BaO + 8 Y_2O_3 + 4SiO_2) {BaO [−3,511 kJ mol^{-1} (Zollweg, 1955)], Y_2O_3 [−15,287 kJ mol^{-1} (Coduri *et al.*, 2013)], SiO_2 [−15,298 kJ mol^{-1} (Smith & Alexander, 1963)]} is 0.5%.

3. Database survey

The ICSD database (ICSD, 2022) contains crystal-structure data for $BaY_2Si_3O_{10}$ (space group $P12_1/m1$) (Kolitsch *et al.*, 2006; Shi *et al.*, 2018), $Ba_9Y_2Si_6O_{24}$ (space group $R\bar{3}$) (Brgoch *et al.*, 2013) and $BaY_4Si_5O_{17}$ (space group $P12_1/m1$) (Wierzbicka-Wieczorek *et al.*, 2015). Lattice constants and space group $I\bar{4}2m$ were reported for $Ba_{5.2}Y_{13}Si_8O_{41}$ (Wierzbicka-Wieczorek *et al.*, 2011). For $Ba_2Y_2Si_4O_{13}$, the structure was described as isomorphic to $Ba_2Gd_2Si_4O_{13}$ (space group $C12/c1$), but lattice parameters were not reported (Song *et al.*, 2019).

4. Synthesis and crystallization

$BaCO_3$ (98% purity, Hakushin Chemical Laboratory), Y_2O_3 (99.99% purity, Shin-Etsu Chemical), and SiO_2 (99.999%

Table 1
Selected bond lengths (Å).

Ba1—O17	2.7478 (17)	Y9—O17	2.3963 (17)
Ba1—O11^{i}	2.7696 (19)	Y9—O14	2.4017 (17)
Ba1—O19	2.7793 (17)	Y10—O16	2.1430 (16)
Ba1—O14	2.8395 (17)	Y10—O26	2.2131 (16)
Ba1—O32^{ii}	2.8661 (18)	Y10—O21	2.2207 (16)
Ba1—O8	2.9444 (17)	Y10—O25	2.3482 (16)
Ba1—O3	2.9600 (17)	Y10—O14	2.4055 (16)
Ba1—O5	3.0333 (18)	Y10—O19	2.4223 (16)
Ba1—O4^{i}	3.0551 (19)	Y11—O20	2.2790 (16)
Ba1—O12	3.1141 (18)	Y11—O16	2.2876 (16)
Ba1—O2^{i}	3.1369 (19)	Y11—O28^{ix}	2.3342 (16)
Ba1—O31^{ii}	3.274 (2)	Y11—O23	2.3374 (16)
Y1—O16	2.2005 (16)	Y11—O9	2.3637 (16)
Y1—O33^{ii}	2.2170 (16)	Y11—O26	2.3799 (16)
Y1—O7^{i}	2.2498 (16)	Y11—O30	2.5071 (16)
Y1—O9	2.3055 (16)	Y12—O24	2.1194 (16)
Y1—O1^{iii}	2.3079 (16)	Y12—O28	2.1921 (16)
Y1—O3	2.5694 (17)	Y12—O29	2.2564 (16)
Y2—O15	2.1496 (16)	Y12—O25	2.2959 (16)
Y2—O13^{iv}	2.1736 (16)	Y12—O19	2.4673 (17)
Y2—O10	2.2282 (16)	Y12—O17	2.4859 (17)
Y2—O6^{iv}	2.3233 (17)	Y13—O27	2.2879 (16)
Y2—O5	2.3485 (17)	Y13—O26	2.2892 (16)
Y2—O2^{i}	2.5253 (18)	Y13—O15^{ix}	2.3290 (16)
Y3—O7	2.2297 (16)	Y13—O10^{ix}	2.3466 (16)
Y3—O7^{v}	2.2436 (17)	Y13—O29	2.3585 (16)
Y3—O9^{vi}	2.2546 (16)	Y13—O23	2.4039 (16)
Y3—O1^{v}	2.2620 (16)	Y13—O18	2.4563 (17)
Y3—O28^{vii}	2.3197 (17)	Y14—O20^{x}	2.2389 (15)
Y3—O8^{v}	2.4654 (17)	Y14—O33	2.2856 (16)
Y4—O1^{iv}	2.1898 (16)	Y14—O7^{ix}	2.2879 (16)
Y4—O29^{viii}	2.2225 (16)	Y14—O24^{iii}	2.3189 (16)
Y4—O10	2.2772 (16)	Y14—O20	2.3499 (16)
Y4—O11	2.2894 (19)	Y14—O28^{iii}	2.3810 (16)
Y4—O6^{iv}	2.3810 (17)	Y14—O30	2.5306 (16)
Y4—O12^{iv}	2.4084 (17)	Y15—O33	2.2050 (16)
Y5—O9	2.1569 (16)	Y15—O27^{iii}	2.2231 (16)
Y5—O13	2.2115 (15)	Y15—O24^{iii}	2.2812 (16)
Y5—O23	2.2252 (16)	Y15—O21	2.3529 (16)
Y5—O18	2.3281 (16)	Y15—O29^{iii}	2.3660 (16)
Y5—O32^{ix}	2.3295 (17)	Y15—O31	2.4990 (19)
Y5—O5^{i}	2.4652 (18)	Y15—O4^{ix}	2.5259 (19)
Y6—O10	2.1976 (16)	Y16—O27^{iii}	2.1983 (16)
Y6—O33^{viii}	2.2074 (16)	Y16—O13^{viii}	2.2097 (16)
Y6—O26^{viii}	2.2225 (16)	Y16—O22^{xi}	2.3185 (16)
Y6—O31^{viii}	2.3284 (18)	Y16—O22	2.3304 (16)
Y6—O30^{viii}	2.3395 (17)	Y16—O15^{xi}	2.3343 (16)
Y6—O3^{iv}	2.4547 (17)	Y16—O2^{ix}	2.5198 (18)
Y7—O24	2.2120 (16)	Y16—O32	2.6127 (17)
Y7—O20^{vi}	2.2383 (16)	Si1—O4^{i}	1.6218 (19)
Y7—O16^{vi}	2.2964 (16)	Si1—O6^{iii}	1.6274 (17)
Y7—O1	2.3113 (16)	Si1—O14	1.6423 (18)
Y7—O21^{vi}	2.3455 (16)	Si1—O2^{i}	1.6428 (18)
Y7—O8	2.5336 (17)	Si2—O18	1.6205 (17)
Y7—O12	2.6233 (17)	Si2—O19	1.6356 (17)
Y8—O21^{vi}	2.2060 (16)	Si2—O3	1.6422 (18)
Y8—O27	2.2339 (16)	Si2—O12	1.6441 (18)
Y8—O13	2.2527 (16)	Si3—O30^{viii}	1.6198 (17)
Y8—O22^{vi}	2.2630 (16)	Si3—O8	1.6277 (17)
Y8—O18	2.3772 (16)	Si3—O17	1.6505 (17)
Y8—O6	2.3887 (17)	Si3—O5	1.6596 (18)
Y9—O15	2.1739 (16)	Si4—O31	1.6201 (18)
Y9—O23^{viii}	2.1745 (16)	Si4—O11^{ix}	1.621 (2)
Y9—O22	2.2201 (16)	Si4—O32	1.6240 (17)
Y9—O25	2.2847 (16)	Si4—O25	1.6276 (17)

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x, -y+1, -z+1$; (vi) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (vii) $-x+1, -y+1, -z+1$; (viii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ix) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (x) $-x+1, -y, -z$; (xi) $-x+1, -y+1, -z$.

purity, Mitsuwa Chemicals) were used as starting materials. Each powder was heated at 1273 K for 5 h and kept in an oven at 453 K. The powders were weighed in a molar ratio of Ba:Y:Si = 1:16:4 and mixed in an agate mortar; the mixed powder was then placed in a mold and formed into disks 5 mm in diameter by uniaxial pressing at ∼60 MPa. The disk was crumbled, and pieces of the fragment were placed on a Pt–Rh plate that was, in turn, placed in an alumina crucible with a lid. The crucible was heated in an electric furnace to 1373 K in air for 3 h; the furnace temperature was then raised from 1373 to 2073 K over a period of 4 h and held at this temperature for 0.5 h. The sample was cooled to room temperature, and a solidified melt was obtained. The sample was crushed, and single crystals were collected from the resulting fragments.

The sample used for powder X-ray diffraction (XRD) analysis was prepared by weighing and mixing the starting materials to obtain a stoichiometric composition of $BaY_{16}Si_4O_{33}$ (Ba:Y:Si molar ratio = 1:16:4). The powder was compacted into a disk shape and heated in an electric furnace from room temperature to 1373 K over a period of 3 h, heated from 1373 to 1793 K over a period of 3 h, maintained at this temperature for 24 h, and then cooled. The resultant polycrystalline ceramic of $BaY_{16}Si_4O_{33}$ was ground in an agate mortar to obtain a powdered sample. The powder XRD pattern was recorded at room temperature using a powder X-ray diffractometer (Bruker AXS, D2PHASER; Fig. S4) equipped with a Cu $K\alpha$ radiation (λ = 1.5418 Å) source. Diffraction patterns were recorded in the diffraction-angle range $5^\circ \leq 2\theta \leq 140^\circ$ with a step interval of 0.025° and a measurement time of 8 s step^{-1}. The obtained XRD pattern was analyzed by the Rietveld method with the program *TOPAS* (Bruker, 2009) using the model determined by single-crystal X-ray structure analysis (Fig. S4 and Table S1) (R_{wp} = 3.03%, R_B = 0.752%). The refined lattice constants [a = 9.11234 (8) Å, b = 18.73111 (19) Å, c = 18.31827 (17) Å, β = 109.0441 (7)°] and atomic positions were close to those obtained from the single-crystal structure analysis (Table S2). The composition of BaO: 8.5 (4), Y_2O_3: 81 (1), SiO_2: 10.6 (2) mass%, which is approximately consistent with the formula $BaY_{16}Si_4O_{33}$ (BaO: 7.0, Y_2O_3: 82.1, SiO_2: 10.9 mass%), was determined by electron-probe microanalysis (EPMA, JEOL A-8200) using a surface-polished and carbon-coated ceramic sample.

Polycrystalline ceramic samples for measurements of the thermal expansion coefficients and dielectric constants were prepared by heating compacted disks of the starting powder mixture with a stoichiometric metal ratio Ba:Y:Si = 1:16:4 at 1793 K for 24 h. The obtained disks were pulverized, and the powder was compacted and heated again under the same conditions. The resultant disks were pulverized and then compacted into a cuboid for measurement of their thermal expansion coefficient and into a disk shape for measurement of their dielectric constant. These compacts were heated at 1953 K for 12 h. The thermal expansion coefficient was measured using a dilatometer (Netzsch Japan, TD5000SA). The capacitance C and dielectric loss tan δ were measured using an LCR meter (HIOKI, IM3536) for the disk sample (96% relative density) with Au electrodes prepared by baking Au paste at 800°C.

Table 2
Experimental details.

Crystal data	
Chemical formula	$BaY_{16}Si_4O_{33}$
M_r	2200.26
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	300
a, b, c (Å)	9.1095 (2), 18.7306 (4), 18.3105 (4)
β (°)	109.008 (1)
V (Å^3)	2953.90 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	32.60
Crystal size (mm)	0.09 × 0.08 × 0.04
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
T_{min}, T_{max}	0.037, 0.094
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	128151, 8279, 7469
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.694
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.016, 0.034, 1.07
No. of reflections	8279
No. of parameters	488
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, −0.90

Computer programs: *BIS* (Bruker, 2018), *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2018), *SHELXT2015* (Sheldrick, 2015*a*), *SHELXL2015* (Sheldrick, 2015*b*), and *VESTA* (Momma & Izumi, 2011)

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atomic coordinates, equivalent isotropic displacement parameters and anisotropic displacement parameters are given in the supporting information.

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supporting information

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$BaY_{16}Si_4O_{33}$ containing $Ba(SiO_4)_4$ orthosilicates

Shuto Motozawa, Hiromitsu Kimura, Junichi Takahashi, Rayko Simura and Hisanori Yamane

Computing details

Data collection: *BIS* (Bruker, 2018); cell refinement: *APEX3* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: *SHELXT2015* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2015* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011).

Barium hexadecayttrium tetrasilicon tritriacontaoxide

Crystal data

$BaY_{16}Si_4O_{33}$
M_r = 2200.26
Monoclinic, $P2_1/c$
a = 9.1095 (2) Å
b = 18.7306 (4) Å
c = 18.3105 (4) Å
β = 109.008 (1)°
V = 2953.90 (11) Å^3
Z = 4
$F(000)$ = 4000
D_x = 4.948 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 120 reflections
θ = 6.9–30.7°
μ = 32.60 mm^{-1}
T = 300 K
Prismatic, translucent colourless
0.09 × 0.08 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: micro focus sealed tube
Detector resolution: 7.3910 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
T_{min} = 0.037, T_{max} = 0.094
128151 measured reflections
8279 independent reflections
7469 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 29.6°, θ_{min} = 2.2°
h = −12→12
k = −26→26
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.034
S = 1.07
8279 reflections
488 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0053P)^2 + 3.9938P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}
Extinction correction: SHELXL-2017/1 (Sheldrick 2015b)
Extinction coefficient: 0.000458 (14)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ba1	0.05096 (2)	0.34871 (2)	0.21348 (2)	0.01140 (3)
Y1	0.02577 (3)	0.14161 (2)	0.08564 (2)	0.00889 (4)
Y2	0.04208 (3)	0.55228 (2)	0.10929 (2)	0.00978 (4)
Y3	0.06456 (3)	0.54810 (2)	0.58895 (2)	0.00912 (4)
Y4	0.07501 (3)	0.75067 (2)	0.11164 (2)	0.00919 (4)
Y5	0.21458 (3)	0.03182 (2)	0.28469 (2)	0.00892 (4)
Y6	0.21892 (3)	0.65949 (2)	0.30143 (2)	0.00932 (4)
Y7	0.28387 (3)	0.34616 (2)	0.47068 (2)	0.00820 (4)
Y8	0.33165 (3)	0.14258 (2)	0.46043 (2)	0.00887 (4)
Y9	0.39522 (3)	0.44733 (2)	0.15331 (2)	0.00900 (4)
Y10	0.40049 (3)	0.24990 (2)	0.14656 (2)	0.00889 (4)
Y11	0.40726 (3)	0.05855 (2)	0.14981 (2)	0.00802 (4)
Y12	0.52776 (3)	0.34670 (2)	0.33477 (2)	0.00940 (4)
Y13	0.59233 (3)	0.13725 (2)	0.33939 (2)	0.00793 (4)
Y14	0.65146 (2)	0.06006 (2)	0.01018 (2)	0.00798 (4)
Y15	0.65622 (3)	0.24911 (2)	0.01128 (2)	0.00842 (4)
Y16	0.68494 (2)	0.45394 (2)	0.02227 (2)	0.00852 (4)
Si1	0.04708 (7)	0.35119 (3)	0.04451 (4)	0.00844 (11)
Si2	0.21185 (7)	0.21283 (3)	0.29091 (4)	0.00787 (11)
Si3	0.21308 (7)	0.47988 (3)	0.30422 (4)	0.00811 (11)
Si4	0.71110 (7)	0.34341 (3)	0.20491 (4)	0.00886 (11)
O1	0.02416 (19)	0.34345 (8)	0.46027 (9)	0.0087 (3)
O2	0.0293 (2)	0.92849 (10)	0.44535 (11)	0.0184 (4)
O3	0.0538 (2)	0.19082 (9)	0.22050 (10)	0.0140 (3)
O4	0.0610 (2)	0.78439 (10)	0.44866 (11)	0.0197 (4)
O5	0.0615 (2)	0.50967 (10)	0.23272 (10)	0.0155 (3)
O6	0.0702 (2)	0.15333 (9)	0.46016 (9)	0.0121 (3)
O7	0.09118 (19)	0.54121 (9)	0.47234 (9)	0.0106 (3)
O8	0.1498 (2)	0.42907 (9)	0.35965 (10)	0.0123 (3)
O9	0.15764 (19)	0.04903 (8)	0.16211 (9)	0.0096 (3)
O10	0.16254 (19)	0.64694 (8)	0.17595 (9)	0.0097 (3)
O11	0.1635 (2)	0.83162 (11)	0.20990 (11)	0.0241 (4)
O12	0.1654 (2)	0.25295 (9)	0.36021 (10)	0.0142 (3)
O13	0.20274 (18)	0.04431 (8)	0.40274 (9)	0.0082 (3)
O14	0.22185 (19)	0.34823 (9)	0.10856 (10)	0.0122 (3)
O15	0.26570 (18)	0.53999 (9)	0.09494 (9)	0.0096 (3)
O16	0.26979 (19)	0.15764 (8)	0.09357 (9)	0.0092 (3)
O17	0.3161 (2)	0.42989 (9)	0.26470 (10)	0.0120 (3)
O18	0.31663 (19)	0.14382 (8)	0.32837 (9)	0.0105 (3)

O19	0.31924 (19)	0.26628 (9)	0.25893 (9)	0.0111 (3)
O20	0.40515 (19)	0.05377 (8)	0.02510 (9)	0.0091 (3)
O21	0.41112 (19)	0.25876 (8)	0.02745 (9)	0.0102 (3)
O22	0.44583 (19)	0.44667 (8)	0.04263 (9)	0.0099 (3)
O23	0.45573 (18)	0.03137 (8)	0.28014 (9)	0.0098 (3)
O24	0.50650 (19)	0.34326 (8)	0.44659 (9)	0.0097 (3)
O25	0.53739 (18)	0.35011 (8)	0.21108 (9)	0.0096 (3)
O26	0.54671 (19)	0.16143 (8)	0.21134 (9)	0.0096 (3)
O27	0.57760 (19)	0.14377 (8)	0.46158 (9)	0.0092 (3)
O28	0.66921 (19)	0.44072 (8)	0.38329 (9)	0.0103 (3)
O29	0.67975 (19)	0.25219 (8)	0.38636 (9)	0.0100 (3)
O30	0.68286 (19)	0.04695 (9)	0.15203 (9)	0.0110 (3)
O31	0.7075 (2)	0.27406 (9)	0.15147 (11)	0.0190 (4)
O32	0.7519 (2)	0.41584 (9)	0.16672 (10)	0.0134 (3)
O33	0.77970 (19)	0.15657 (8)	0.07783 (9)	0.0085 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01007 (6)	0.01158 (6)	0.01264 (7)	0.00016 (5)	0.00381 (5)	0.00013 (5)
Y1	0.00706 (10)	0.01126 (10)	0.00829 (10)	−0.00009 (8)	0.00242 (8)	−0.00038 (7)
Y2	0.00673 (10)	0.00988 (10)	0.01212 (10)	0.00019 (8)	0.00223 (8)	−0.00088 (8)
Y3	0.00828 (10)	0.00970 (9)	0.00923 (10)	0.00122 (8)	0.00264 (8)	0.00187 (8)
Y4	0.00750 (10)	0.00867 (9)	0.01056 (10)	0.00052 (8)	0.00178 (8)	0.00148 (8)
Y5	0.00866 (10)	0.01055 (10)	0.00723 (9)	−0.00086 (8)	0.00217 (8)	−0.00042 (7)
Y6	0.00816 (10)	0.01254 (10)	0.00706 (9)	0.00077 (8)	0.00223 (8)	0.00055 (7)
Y7	0.00724 (10)	0.00913 (9)	0.00804 (9)	−0.00020 (8)	0.00224 (7)	−0.00029 (7)
Y8	0.00789 (10)	0.00854 (9)	0.01006 (10)	−0.00088 (8)	0.00273 (8)	−0.00153 (7)
Y9	0.01067 (10)	0.00790 (9)	0.00788 (9)	0.00026 (8)	0.00226 (8)	0.00023 (7)
Y10	0.01035 (10)	0.00768 (9)	0.00781 (10)	−0.00013 (7)	0.00182 (8)	−0.00046 (7)
Y11	0.00807 (10)	0.00840 (9)	0.00715 (9)	−0.00019 (7)	0.00186 (7)	−0.00013 (7)
Y12	0.01153 (10)	0.00896 (9)	0.00710 (9)	−0.00063 (8)	0.00222 (8)	−0.00024 (7)
Y13	0.00789 (10)	0.00852 (9)	0.00716 (9)	−0.00028 (7)	0.00215 (7)	−0.00015 (7)
Y14	0.00767 (10)	0.00776 (9)	0.00807 (9)	−0.00032 (7)	0.00196 (7)	−0.00037 (7)
Y15	0.00900 (10)	0.00763 (9)	0.00850 (9)	0.00073 (7)	0.00266 (8)	0.00070 (7)
Y16	0.00846 (10)	0.00831 (9)	0.00839 (9)	−0.00055 (8)	0.00221 (8)	−0.00087 (7)
Si1	0.0082 (3)	0.0095 (3)	0.0074 (3)	−0.0004 (2)	0.0021 (2)	0.0001 (2)
Si2	0.0074 (3)	0.0080 (3)	0.0078 (3)	0.0001 (2)	0.0020 (2)	0.0005 (2)
Si3	0.0081 (3)	0.0082 (3)	0.0078 (3)	−0.0006 (2)	0.0024 (2)	−0.0003 (2)
Si4	0.0077 (3)	0.0089 (3)	0.0098 (3)	0.0004 (2)	0.0026 (2)	0.0016 (2)
O1	0.0095 (8)	0.0092 (7)	0.0075 (7)	0.0002 (6)	0.0027 (6)	−0.0005 (6)
O2	0.0129 (9)	0.0146 (8)	0.0244 (10)	−0.0032 (7)	0.0017 (7)	0.0048 (7)
O3	0.0102 (8)	0.0183 (9)	0.0112 (8)	−0.0022 (7)	0.0006 (6)	−0.0022 (7)
O4	0.0168 (9)	0.0195 (9)	0.0230 (10)	0.0051 (7)	0.0069 (8)	−0.0031 (8)
O5	0.0118 (8)	0.0212 (9)	0.0121 (8)	0.0018 (7)	0.0020 (7)	0.0048 (7)
O6	0.0113 (8)	0.0156 (8)	0.0087 (8)	0.0005 (6)	0.0022 (6)	0.0004 (6)
O7	0.0086 (8)	0.0130 (8)	0.0094 (8)	−0.0008 (6)	0.0017 (6)	0.0004 (6)
O8	0.0127 (8)	0.0119 (8)	0.0135 (8)	0.0001 (6)	0.0058 (6)	0.0020 (6)

O9	0.0092 (8)	0.0104 (7)	0.0085 (7)	−0.0016 (6)	0.0017 (6)	−0.0010 (6)
O10	0.0099 (8)	0.0099 (7)	0.0083 (7)	0.0003 (6)	0.0018 (6)	−0.0008 (6)
O11	0.0132 (9)	0.0377 (12)	0.0181 (9)	0.0014 (8)	0.0005 (7)	−0.0145 (8)
O12	0.0133 (9)	0.0170 (8)	0.0147 (8)	−0.0021 (7)	0.0077 (7)	−0.0038 (7)
O13	0.0084 (7)	0.0085 (7)	0.0073 (7)	−0.0001 (6)	0.0020 (6)	−0.0002 (6)
O14	0.0092 (8)	0.0126 (8)	0.0113 (8)	0.0008 (6)	−0.0016 (6)	−0.0013 (6)
O15	0.0085 (8)	0.0108 (7)	0.0097 (7)	0.0008 (6)	0.0031 (6)	0.0004 (6)
O16	0.0081 (8)	0.0099 (7)	0.0093 (7)	0.0003 (6)	0.0026 (6)	0.0001 (6)
O17	0.0125 (8)	0.0121 (8)	0.0125 (8)	0.0015 (6)	0.0054 (6)	−0.0004 (6)
O18	0.0102 (8)	0.0092 (7)	0.0111 (8)	−0.0002 (6)	0.0021 (6)	0.0011 (6)
O19	0.0128 (8)	0.0109 (7)	0.0107 (8)	−0.0021 (6)	0.0053 (6)	0.0001 (6)
O20	0.0105 (8)	0.0077 (7)	0.0089 (7)	−0.0011 (6)	0.0028 (6)	−0.0006 (6)
O21	0.0115 (8)	0.0091 (7)	0.0110 (8)	0.0004 (6)	0.0049 (6)	0.0013 (6)
O22	0.0092 (8)	0.0114 (8)	0.0097 (7)	0.0003 (6)	0.0038 (6)	−0.0004 (6)
O23	0.0081 (8)	0.0121 (8)	0.0086 (7)	−0.0005 (6)	0.0021 (6)	0.0011 (6)
O24	0.0081 (8)	0.0112 (7)	0.0099 (7)	−0.0003 (6)	0.0030 (6)	0.0005 (6)
O25	0.0081 (8)	0.0108 (7)	0.0094 (7)	0.0004 (6)	0.0019 (6)	0.0004 (6)
O26	0.0084 (8)	0.0108 (7)	0.0088 (7)	0.0003 (6)	0.0020 (6)	0.0003 (6)
O27	0.0099 (8)	0.0091 (7)	0.0086 (7)	−0.0002 (6)	0.0032 (6)	−0.0009 (6)
O28	0.0104 (8)	0.0104 (7)	0.0091 (7)	−0.0017 (6)	0.0020 (6)	0.0001 (6)
O29	0.0093 (8)	0.0099 (7)	0.0107 (8)	0.0003 (6)	0.0031 (6)	0.0005 (6)
O30	0.0103 (8)	0.0109 (7)	0.0111 (8)	0.0023 (6)	0.0024 (6)	0.0025 (6)
O31	0.0301 (11)	0.0097 (8)	0.0221 (10)	0.0016 (7)	0.0153 (8)	−0.0009 (7)
O32	0.0161 (9)	0.0114 (8)	0.0130 (8)	−0.0029 (7)	0.0052 (7)	0.0014 (6)
O33	0.0082 (7)	0.0086 (7)	0.0082 (7)	0.0002 (6)	0.0019 (6)	−0.0003 (6)

Geometric parameters (Å, º)

Ba1—O17	2.7478 (17)	Y8—O12	2.8503 (18)
Ba1—O11^{i}	2.7696 (19)	Y9—O15	2.1739 (16)
Ba1—O19	2.7793 (17)	Y9—O23^{viii}	2.1745 (16)
Ba1—O14	2.8395 (17)	Y9—O22	2.2201 (16)
Ba1—O32^{ii}	2.8661 (18)	Y9—O25	2.2847 (16)
Ba1—O8	2.9444 (17)	Y9—O17	2.3963 (17)
Ba1—O3	2.9600 (17)	Y9—O14	2.4017 (17)
Ba1—O5	3.0333 (18)	Y10—O16	2.1430 (16)
Ba1—Si2	3.0467 (6)	Y10—O26	2.2131 (16)
Ba1—Si4^{ii}	3.0500 (7)	Y10—O21	2.2207 (16)
Ba1—O4^{i}	3.0551 (19)	Y10—O25	2.3482 (16)
Ba1—Si3	3.0626 (6)	Y10—O14	2.4055 (16)
Ba1—Si1	3.0831 (6)	Y10—O19	2.4223 (16)
Ba1—O12	3.1141 (18)	Y10—O31	2.8058 (19)
Ba1—O2^{i}	3.1369 (19)	Y11—O20	2.2790 (16)
Ba1—O31^{ii}	3.274 (2)	Y11—O16	2.2876 (16)
Ba1—Y9	4.0878 (3)	Y11—O28^{ix}	2.3342 (16)
Ba1—Y4^{i}	4.1637 (3)	Y11—O23	2.3374 (16)
Ba1—Y12	4.1851 (3)	Y11—O9	2.3637 (16)
Ba1—Y10	4.1960 (3)	Y11—O26	2.3799 (16)

Y1—O16	2.2005 (16)	Y11—O30	2.5071 (16)
Y1—O33^{ii}	2.2170 (16)	Y12—O24	2.1194 (16)
Y1—O7^{i}	2.2498 (16)	Y12—O28	2.1921 (16)
Y1—O9	2.3055 (16)	Y12—O29	2.2564 (16)
Y1—O1^{iii}	2.3079 (16)	Y12—O25	2.2959 (16)
Y1—O3	2.5694 (17)	Y12—O19	2.4673 (17)
Y1—O4^{i}	2.8014 (19)	Y12—O17	2.4859 (17)
Y1—Y14^{ii}	3.5777 (3)	Y13—O27	2.2879 (16)
Y1—Y11	3.6356 (3)	Y13—O26	2.2892 (16)
Y2—O15	2.1496 (16)	Y13—O15^{ix}	2.3290 (16)
Y2—O13^{iv}	2.1736 (16)	Y13—O10^{ix}	2.3466 (16)
Y2—O10	2.2282 (16)	Y13—O29	2.3585 (16)
Y2—O6^{iv}	2.3233 (17)	Y13—O23	2.4039 (16)
Y2—O5	2.3485 (17)	Y13—O18	2.4563 (17)
Y2—O2^{i}	2.5253 (18)	Y14—O20^{x}	2.2389 (15)
Y3—O7	2.2297 (16)	Y14—O33	2.2856 (16)
Y3—O7^{v}	2.2436 (17)	Y14—O7^{ix}	2.2879 (16)
Y3—O9^{vi}	2.2546 (16)	Y14—O24^{iii}	2.3189 (16)
Y3—O1^{v}	2.2620 (16)	Y14—O20	2.3499 (16)
Y3—O28^{vii}	2.3197 (17)	Y14—O28^{iii}	2.3810 (16)
Y3—O8^{v}	2.4654 (17)	Y14—O30	2.5306 (16)
Y4—O1^{iv}	2.1898 (16)	Y15—O33	2.2050 (16)
Y4—O29^{viii}	2.2225 (16)	Y15—O27^{iii}	2.2231 (16)
Y4—O10	2.2772 (16)	Y15—O24^{iii}	2.2812 (16)
Y4—O11	2.2894 (19)	Y15—O21	2.3529 (16)
Y4—O6^{iv}	2.3810 (17)	Y15—O29^{iii}	2.3660 (16)
Y4—O12^{iv}	2.4084 (17)	Y15—O31	2.4990 (19)
Y5—O9	2.1569 (16)	Y15—O4^{ix}	2.5259 (19)
Y5—O13	2.2115 (15)	Y16—O27^{iii}	2.1983 (16)
Y5—O23	2.2252 (16)	Y16—O13^{viii}	2.2097 (16)
Y5—O18	2.3281 (16)	Y16—O22^{xi}	2.3185 (16)
Y5—O32^{ix}	2.3295 (17)	Y16—O22	2.3304 (16)
Y5—O5^{i}	2.4652 (18)	Y16—O15^{xi}	2.3343 (16)
Y6—O10	2.1976 (16)	Y16—O2^{ix}	2.5198 (18)
Y6—O33^{viii}	2.2074 (16)	Y16—O32	2.6127 (17)
Y6—O26^{viii}	2.2225 (16)	Si1—O4^{i}	1.6218 (19)
Y6—O31^{viii}	2.3284 (18)	Si1—O6^{iii}	1.6274 (17)
Y6—O30^{viii}	2.3395 (17)	Si1—O14	1.6423 (18)
Y6—O3^{iv}	2.4547 (17)	Si1—O2^{i}	1.6428 (18)
Y7—O24	2.2120 (16)	Si2—O18	1.6205 (17)
Y7—O20^{vi}	2.2383 (16)	Si2—O19	1.6356 (17)
Y7—O16^{vi}	2.2964 (16)	Si2—O3	1.6422 (18)
Y7—O1	2.3113 (16)	Si2—O12	1.6441 (18)
Y7—O21^{vi}	2.3455 (16)	Si3—O30^{viii}	1.6198 (17)
Y7—O8	2.5336 (17)	Si3—O8	1.6277 (17)
Y7—O12	2.6233 (17)	Si3—O17	1.6505 (17)
Y8—O21^{vi}	2.2060 (16)	Si3—O5	1.6596 (18)
Y8—O27	2.2339 (16)	Si4—O31	1.6201 (18)

Y8—O13	2.2527 (16)	Si4—O11^{ix}	1.621 (2)
Y8—O22^{vi}	2.2630 (16)	Si4—O32	1.6240 (17)
Y8—O18	2.3772 (16)	Si4—O25	1.6276 (17)
Y8—O6	2.3887 (17)		

O17—Ba1—O11^{i}	125.29 (6)	O15^{ix}—Y13—O18	117.55 (5)
O17—Ba1—O19	67.40 (5)	O10^{ix}—Y13—O18	166.82 (5)
O11^{i}—Ba1—O19	118.72 (5)	O29—Y13—O18	101.48 (5)
O17—Ba1—O14	67.54 (5)	O23—Y13—O18	68.84 (5)
O11^{i}—Ba1—O14	167.12 (5)	O20^{x}—Y14—O33	159.82 (6)
O19—Ba1—O14	65.07 (5)	O20^{x}—Y14—O7^{ix}	91.30 (6)
O17—Ba1—O32^{ii}	120.23 (5)	O33—Y14—O7^{ix}	74.14 (6)
O11^{i}—Ba1—O32^{ii}	56.19 (5)	O20^{x}—Y14—O24^{iii}	123.98 (6)
O19—Ba1—O32^{ii}	172.15 (5)	O33—Y14—O24^{iii}	76.20 (6)
O14—Ba1—O32^{ii}	118.45 (5)	O7^{ix}—Y14—O24^{iii}	125.50 (6)
O17—Ba1—O8	55.42 (5)	O20^{x}—Y14—O20	81.19 (6)
O11^{i}—Ba1—O8	69.87 (5)	O33—Y14—O20	108.39 (6)
O19—Ba1—O8	91.90 (5)	O7^{ix}—Y14—O20	161.75 (6)
O14—Ba1—O8	122.96 (5)	O24^{iii}—Y14—O20	71.84 (5)
O32^{ii}—Ba1—O8	91.53 (5)	O20^{x}—Y14—O28^{iii}	78.17 (6)
O17—Ba1—O3	122.95 (5)	O33—Y14—O28^{iii}	110.40 (6)
O11^{i}—Ba1—O3	81.95 (6)	O7^{ix}—Y14—O28^{iii}	75.13 (6)
O19—Ba1—O3	55.78 (5)	O24^{iii}—Y14—O28^{iii}	73.94 (5)
O14—Ba1—O3	91.56 (5)	O20—Y14—O28^{iii}	118.95 (6)
O32^{ii}—Ba1—O3	116.44 (5)	O20^{x}—Y14—O30	98.17 (5)
O8—Ba1—O3	118.40 (5)	O33—Y14—O30	69.73 (5)
O17—Ba1—O5	54.50 (5)	O7^{ix}—Y14—O30	94.20 (5)
O11^{i}—Ba1—O5	93.27 (6)	O24^{iii}—Y14—O30	116.53 (5)
O19—Ba1—O5	121.73 (5)	O20—Y14—O30	70.66 (5)
O14—Ba1—O5	94.48 (5)	O28^{iii}—Y14—O30	168.52 (5)
O32^{ii}—Ba1—O5	65.78 (5)	O33—Y15—O27^{iii}	166.92 (6)
O8—Ba1—O5	52.96 (5)	O33—Y15—O24^{iii}	78.57 (6)
O3—Ba1—O5	171.32 (5)	O27^{iii}—Y15—O24^{iii}	114.43 (6)
O17—Ba1—O4^{i}	121.87 (5)	O33—Y15—O21	108.96 (6)
O11^{i}—Ba1—O4^{i}	112.30 (5)	O27^{iii}—Y15—O21	77.87 (6)
O19—Ba1—O4^{i}	93.13 (5)	O24^{iii}—Y15—O21	72.07 (6)
O14—Ba1—O4^{i}	54.85 (5)	O33—Y15—O29^{iii}	109.61 (6)
O32^{ii}—Ba1—O4^{i}	84.19 (5)	O27^{iii}—Y15—O29^{iii}	74.46 (6)
O8—Ba1—O4^{i}	172.47 (5)	O24^{iii}—Y15—O29^{iii}	73.58 (6)
O3—Ba1—O4^{i}	69.12 (5)	O21—Y15—O29^{iii}	120.73 (6)
O5—Ba1—O4^{i}	119.52 (5)	O33—Y15—O31	71.83 (6)
O17—Ba1—O12	90.81 (5)	O27^{iii}—Y15—O31	100.32 (6)
O11^{i}—Ba1—O12	65.77 (5)	O24^{iii}—Y15—O31	123.73 (6)
O19—Ba1—O12	53.63 (4)	O21—Y15—O31	73.98 (6)
O14—Ba1—O12	118.59 (5)	O29^{iii}—Y15—O31	161.71 (6)
O32^{ii}—Ba1—O12	121.94 (5)	O33—Y15—O4^{ix}	75.92 (6)
O8—Ba1—O12	65.98 (5)	O27^{iii}—Y15—O4^{ix}	92.57 (6)
O3—Ba1—O12	52.51 (4)	O24^{iii}—Y15—O4^{ix}	136.88 (6)

O5—Ba1—O12	118.90 (5)	O21—Y15—O4^{ix}	149.68 (6)
O4^{i}—Ba1—O12	121.55 (5)	O29^{iii}—Y15—O4^{ix}	83.02 (6)
O17—Ba1—O2^{i}	88.07 (5)	O31—Y15—O4^{ix}	79.68 (6)
O11^{i}—Ba1—O2^{i}	122.33 (5)	O27^{iii}—Y16—O13^{viii}	172.57 (6)
O19—Ba1—O2^{i}	117.32 (5)	O27^{iii}—Y16—O22^{xi}	109.86 (6)
O14—Ba1—O2^{i}	52.26 (5)	O13^{viii}—Y16—O22^{xi}	76.11 (6)
O32^{ii}—Ba1—O2^{i}	66.56 (5)	O27^{iii}—Y16—O22	75.36 (6)
O8—Ba1—O2^{i}	120.61 (5)	O13^{viii}—Y16—O22	102.30 (6)
O3—Ba1—O2^{i}	120.81 (5)	O22^{xi}—Y16—O22	77.17 (6)
O5—Ba1—O2^{i}	67.87 (5)	O27^{iii}—Y16—O15^{xi}	76.29 (6)
O4^{i}—Ba1—O2^{i}	51.95 (5)	O13^{viii}—Y16—O15^{xi}	110.19 (6)
O12—Ba1—O2^{i}	170.28 (4)	O22^{xi}—Y16—O15^{xi}	73.17 (6)
O17—Ba1—O31^{ii}	171.58 (5)	O22—Y16—O15^{xi}	128.31 (6)
O11^{i}—Ba1—O31^{ii}	51.27 (5)	O27^{iii}—Y16—O2^{ix}	102.52 (6)
O19—Ba1—O31^{ii}	120.95 (5)	O13^{viii}—Y16—O2^{ix}	76.41 (6)
O14—Ba1—O31^{ii}	115.88 (5)	O22^{xi}—Y16—O2^{ix}	126.26 (6)
O32^{ii}—Ba1—O31^{ii}	51.38 (5)	O22—Y16—O2^{ix}	154.03 (6)
O8—Ba1—O31^{ii}	120.55 (4)	O15^{xi}—Y16—O2^{ix}	74.45 (6)
O3—Ba1—O31^{ii}	65.30 (5)	O27^{iii}—Y16—O32	101.72 (6)
O5—Ba1—O31^{ii}	117.09 (5)	O13^{viii}—Y16—O32	70.85 (5)
O4^{i}—Ba1—O31^{ii}	61.03 (5)	O22^{xi}—Y16—O32	130.53 (5)
O12—Ba1—O31^{ii}	93.83 (5)	O22—Y16—O32	75.19 (5)
O2^{i}—Ba1—O31^{ii}	88.51 (5)	O15^{xi}—Y16—O32	153.20 (6)
O16—Y1—O33^{ii}	164.90 (6)	O2^{ix}—Y16—O32	80.06 (6)
O16—Y1—O7^{i}	117.27 (6)	O4^{i}—Si1—O6^{iii}	107.60 (10)
O33^{ii}—Y1—O7^{i}	76.22 (6)	O4^{i}—Si1—O14	112.98 (10)
O16—Y1—O9	75.36 (6)	O6^{iii}—Si1—O14	106.32 (9)
O33^{ii}—Y1—O9	116.75 (6)	O4^{i}—Si1—O2^{i}	112.40 (10)
O7^{i}—Y1—O9	74.38 (6)	O6^{iii}—Si1—O2^{i}	110.10 (10)
O16—Y1—O1^{iii}	74.23 (6)	O14—Si1—O2^{i}	107.27 (9)
O33^{ii}—Y1—O1^{iii}	103.99 (6)	O18—Si2—O19	107.53 (9)
O7^{i}—Y1—O1^{iii}	77.49 (6)	O18—Si2—O3	112.15 (9)
O9—Y1—O1^{iii}	121.91 (6)	O19—Si2—O3	110.27 (9)
O16—Y1—O3	96.07 (6)	O18—Si2—O12	107.58 (9)
O33^{ii}—Y1—O3	78.37 (6)	O19—Si2—O12	109.31 (9)
O7^{i}—Y1—O3	129.56 (6)	O3—Si2—O12	109.91 (9)
O9—Y1—O3	79.47 (6)	O30^{viii}—Si3—O8	114.47 (9)
O1^{iii}—Y1—O3	151.51 (6)	O30^{viii}—Si3—O17	109.39 (9)
O16—Y1—O4^{i}	95.15 (6)	O8—Si3—O17	108.02 (9)
O33^{ii}—Y1—O4^{i}	70.09 (5)	O30^{viii}—Si3—O5	109.38 (9)
O7^{i}—Y1—O4^{i}	129.53 (6)	O8—Si3—O5	108.41 (9)
O9—Y1—O4^{i}	155.15 (6)	O17—Si3—O5	106.90 (9)
O1^{iii}—Y1—O4^{i}	75.60 (5)	O31—Si4—O11^{ix}	109.95 (11)
O3—Y1—O4^{i}	78.78 (6)	O31—Si4—O32	111.84 (10)
O15—Y2—O13^{iv}	164.19 (6)	O11^{ix}—Si4—O32	109.85 (10)
O15—Y2—O10	80.50 (6)	O31—Si4—O25	105.96 (10)
O13^{iv}—Y2—O10	114.60 (6)	O11^{ix}—Si4—O25	109.90 (10)
O15—Y2—O6^{iv}	106.62 (6)	O32—Si4—O25	109.25 (9)

O13^{iv}—Y2—O6^{iv}	75.30 (6)	Y3^{v}—O1—Y1^{vi}	99.97 (6)
O10—Y2—O6^{iv}	72.67 (6)	Y4^{i}—O1—Y7	106.13 (6)
O15—Y2—O5	107.69 (6)	Y3^{v}—O1—Y7	103.68 (6)
O13^{iv}—Y2—O5	80.07 (6)	Y1^{vi}—O1—Y7	103.92 (6)
O10—Y2—O5	82.76 (6)	Si1^{iv}—O2—Y16^{viii}	125.68 (10)
O6^{iv}—Y2—O5	133.27 (6)	Si1^{iv}—O2—Y2^{iv}	142.19 (10)
O15—Y2—O2^{i}	89.15 (6)	Y16^{viii}—O2—Y2^{iv}	91.86 (6)
O13^{iv}—Y2—O2^{i}	76.91 (6)	Si1^{iv}—O2—Ba1^{iv}	72.88 (7)
O10—Y2—O2^{i}	164.80 (6)	Y16^{viii}—O2—Ba1^{iv}	102.67 (6)
O6^{iv}—Y2—O2^{i}	121.37 (6)	Y2^{iv}—O2—Ba1^{iv}	96.77 (6)
O5—Y2—O2^{i}	89.90 (6)	Si2—O3—Y6^{i}	140.38 (10)
O7—Y3—O7^{v}	74.11 (7)	Si2—O3—Y1	129.18 (9)
O7—Y3—O9^{vi}	112.65 (6)	Y6^{i}—O3—Y1	88.78 (5)
O7^{v}—Y3—O9^{vi}	75.50 (6)	Si2—O3—Ba1	77.07 (7)
O7—Y3—O1^{v}	78.85 (6)	Y6^{i}—O3—Ba1	103.76 (6)
O7^{v}—Y3—O1^{v}	112.62 (6)	Y1—O3—Ba1	108.66 (6)
O9^{vi}—Y3—O1^{v}	167.88 (6)	Si1^{iv}—O4—Y15^{viii}	140.05 (11)
O7—Y3—O28^{vii}	77.47 (6)	Si1^{iv}—O4—Y1^{iv}	128.30 (10)
O7^{v}—Y3—O28^{vii}	128.51 (6)	Y15^{viii}—O4—Y1^{iv}	90.11 (6)
O9^{vi}—Y3—O28^{vii}	77.21 (6)	Si1^{iv}—O4—Ba1^{iv}	75.63 (7)
O1^{v}—Y3—O28^{vii}	102.63 (6)	Y15^{viii}—O4—Ba1^{iv}	111.80 (6)
O7—Y3—O8^{v}	136.24 (6)	Y1^{iv}—O4—Ba1^{iv}	100.26 (6)
O7^{v}—Y3—O8^{v}	82.52 (6)	Si3—O5—Y2	131.00 (10)
O9^{vi}—Y3—O8^{v}	95.99 (6)	Si3—O5—Y5^{iv}	135.25 (9)
O1^{v}—Y3—O8^{v}	76.80 (6)	Y2—O5—Y5^{iv}	93.69 (6)
O28^{vii}—Y3—O8^{v}	143.34 (6)	Si3—O5—Ba1	75.18 (7)
O1^{iv}—Y4—O29^{viii}	102.44 (6)	Y2—O5—Ba1	103.67 (6)
O1^{iv}—Y4—O10	173.96 (6)	Y5^{iv}—O5—Ba1	99.19 (6)
O29^{viii}—Y4—O10	79.72 (6)	Si1^{vi}—O6—Y2^{i}	107.89 (8)
O1^{iv}—Y4—O11	85.27 (7)	Si1^{vi}—O6—Y4^{i}	110.09 (9)
O29^{viii}—Y4—O11	83.33 (6)	Y2^{i}—O6—Y4^{i}	104.79 (7)
O10—Y4—O11	100.62 (7)	Si1^{vi}—O6—Y8	115.51 (9)
O1^{iv}—Y4—O6^{iv}	103.27 (6)	Y2^{i}—O6—Y8	101.15 (6)
O29^{viii}—Y4—O6^{iv}	113.18 (6)	Y4^{i}—O6—Y8	116.09 (7)
O10—Y4—O6^{iv}	70.74 (6)	Y3—O7—Y3^{v}	105.89 (7)
O11—Y4—O6^{iv}	158.61 (7)	Y3—O7—Y1^{iv}	102.77 (7)
O1^{iv}—Y4—O12^{iv}	83.61 (6)	Y3^{v}—O7—Y1^{iv}	105.20 (7)
O29^{viii}—Y4—O12^{iv}	167.30 (6)	Y3—O7—Y14^{viii}	106.45 (7)
O10—Y4—O12^{iv}	95.40 (6)	Y3^{v}—O7—Y14^{viii}	129.59 (8)
O11—Y4—O12^{iv}	86.09 (7)	Y1^{iv}—O7—Y14^{viii}	104.07 (6)
O6^{iv}—Y4—O12^{iv}	75.61 (6)	Si3—O8—Y3^{v}	128.47 (9)
O9—Y5—O13	158.36 (6)	Si3—O8—Y7	133.04 (9)
O9—Y5—O23	82.38 (6)	Y3^{v}—O8—Y7	91.99 (5)
O13—Y5—O23	113.58 (6)	Si3—O8—Ba1	78.32 (7)
O9—Y5—O18	99.01 (6)	Y3^{v}—O8—Ba1	112.96 (6)
O13—Y5—O18	73.14 (6)	Y7—O8—Ba1	109.92 (6)
O23—Y5—O18	74.20 (6)	Y5—O9—Y3^{iii}	114.47 (7)
O9—Y5—O32^{ix}	119.60 (6)	Y5—O9—Y1	130.21 (7)

O13—Y5—O32^{ix}	76.55 (6)	Y3^{iii}—O9—Y1	103.02 (6)
O23—Y5—O32^{ix}	90.16 (6)	Y5—O9—Y11	101.40 (6)
O18—Y5—O32^{ix}	136.15 (6)	Y3^{iii}—O9—Y11	101.04 (6)
O9—Y5—O5^{i}	90.07 (6)	Y1—O9—Y11	102.27 (6)
O13—Y5—O5^{i}	76.80 (6)	Y6—O10—Y2	124.30 (7)
O23—Y5—O5^{i}	166.55 (6)	Y6—O10—Y4	111.88 (7)
O18—Y5—O5^{i}	118.19 (6)	Y2—O10—Y4	111.63 (7)
O32^{ix}—Y5—O5^{i}	83.90 (6)	Y6—O10—Y13^{viii}	103.06 (6)
O10—Y6—O33^{viii}	165.38 (6)	Y2—O10—Y13^{viii}	101.01 (6)
O10—Y6—O26^{viii}	78.30 (6)	Y4—O10—Y13^{viii}	100.99 (6)
O33^{viii}—Y6—O26^{viii}	114.42 (6)	Si4^{viii}—O11—Y4	143.51 (12)
O10—Y6—O31^{viii}	115.27 (6)	Si4^{viii}—O11—Ba1^{iv}	83.64 (8)
O33^{viii}—Y6—O31^{viii}	75.21 (6)	Y4—O11—Ba1^{iv}	110.42 (7)
O26^{viii}—Y6—O31^{viii}	81.58 (6)	Si2—O12—Y4^{i}	129.61 (10)
O10—Y6—O30^{viii}	102.46 (6)	Si2—O12—Y7	139.00 (9)
O33^{viii}—Y6—O30^{viii}	74.70 (6)	Y4^{i}—O12—Y7	91.21 (5)
O26^{viii}—Y6—O30^{viii}	77.67 (6)	Si2—O12—Y8	87.08 (7)
O31^{viii}—Y6—O30^{viii}	131.74 (7)	Y4^{i}—O12—Y8	100.30 (6)
O10—Y6—O3^{iv}	88.57 (6)	Y7—O12—Y8	89.28 (5)
O33^{viii}—Y6—O3^{iv}	81.09 (6)	Si2—O12—Ba1	72.27 (6)
O26^{viii}—Y6—O3^{iv}	159.14 (6)	Y4^{i}—O12—Ba1	97.04 (6)
O31^{viii}—Y6—O3^{iv}	89.66 (6)	Y7—O12—Ba1	102.71 (5)
O30^{viii}—Y6—O3^{iv}	121.43 (6)	Y8—O12—Ba1	158.69 (6)
O24—Y7—O20^{vi}	75.98 (6)	Y2^{i}—O13—Y16^{ix}	111.58 (7)
O24—Y7—O16^{vi}	122.82 (6)	Y2^{i}—O13—Y5	106.46 (7)
O20^{vi}—Y7—O16^{vi}	76.51 (6)	Y16^{ix}—O13—Y5	111.48 (7)
O24—Y7—O1	164.43 (6)	Y2^{i}—O13—Y8	110.63 (7)
O20^{vi}—Y7—O1	113.49 (6)	Y16^{ix}—O13—Y8	105.63 (6)
O16^{vi}—Y7—O1	72.41 (6)	Y5—O13—Y8	111.16 (7)
O24—Y7—O21^{vi}	73.43 (6)	Si1—O14—Y9	126.47 (9)
O20^{vi}—Y7—O21^{vi}	113.78 (6)	Si1—O14—Y10	129.76 (9)
O16^{vi}—Y7—O21^{vi}	73.56 (6)	Y9—O14—Y10	100.68 (6)
O1—Y7—O21^{vi}	111.28 (6)	Si1—O14—Ba1	82.27 (7)
O24—Y7—O8	95.10 (6)	Y9—O14—Ba1	102.19 (6)
O20^{vi}—Y7—O8	83.28 (6)	Y10—O14—Ba1	105.96 (6)
O16^{vi}—Y7—O8	129.72 (6)	Y2—O15—Y9	114.18 (7)
O1—Y7—O8	74.59 (5)	Y2—O15—Y13^{viii}	104.01 (6)
O21^{vi}—Y7—O8	155.33 (6)	Y9—O15—Y13^{viii}	104.44 (7)
O24—Y7—O12	90.20 (6)	Y2—O15—Y16^{xi}	125.53 (7)
O20^{vi}—Y7—O12	156.93 (6)	Y9—O15—Y16^{xi}	104.76 (6)
O16^{vi}—Y7—O12	126.50 (6)	Y13^{viii}—O15—Y16^{xi}	101.29 (6)
O1—Y7—O12	76.64 (5)	Y10—O16—Y1	122.70 (7)
O21^{vi}—Y7—O12	78.69 (6)	Y10—O16—Y11	107.97 (7)
O8—Y7—O12	79.60 (6)	Y1—O16—Y11	108.19 (7)
O21^{vi}—Y8—O27	80.79 (6)	Y10—O16—Y7^{iii}	105.58 (7)
O21^{vi}—Y8—O13	166.37 (6)	Y1—O16—Y7^{iii}	107.98 (7)
O27—Y8—O13	112.37 (6)	Y11—O16—Y7^{iii}	102.64 (6)
O21^{vi}—Y8—O22^{vi}	104.62 (6)	Si3—O17—Y9	131.87 (9)

O27—Y8—O22^{vi}	76.04 (6)	Si3—O17—Y12	125.83 (9)
O13—Y8—O22^{vi}	76.40 (6)	Y9—O17—Y12	97.30 (6)
O21^{vi}—Y8—O18	117.22 (6)	Si3—O17—Ba1	84.34 (7)
O27—Y8—O18	74.62 (6)	Y9—O17—Ba1	105.04 (6)
O13—Y8—O18	71.48 (6)	Y12—O17—Ba1	106.08 (6)
O22^{vi}—Y8—O18	123.05 (6)	Si2—O18—Y5	117.33 (9)
O21^{vi}—Y8—O6	94.41 (6)	Si2—O18—Y8	105.61 (8)
O27—Y8—O6	174.58 (6)	Y5—O18—Y8	103.00 (6)
O13—Y8—O6	72.59 (6)	Si2—O18—Y13	121.35 (9)
O22^{vi}—Y8—O6	107.80 (6)	Y5—O18—Y13	105.44 (6)
O18—Y8—O6	105.67 (6)	Y8—O18—Y13	101.38 (6)
O21^{vi}—Y8—O12	76.10 (6)	Si2—O19—Y10	127.62 (9)
O27—Y8—O12	108.64 (5)	Si2—O19—Y12	127.79 (9)
O13—Y8—O12	101.78 (5)	Y10—O19—Y12	99.39 (6)
O22^{vi}—Y8—O12	175.29 (5)	Si2—O19—Ba1	82.94 (7)
O18—Y8—O12	59.70 (5)	Y10—O19—Ba1	107.35 (6)
O6—Y8—O12	67.50 (5)	Y12—O19—Ba1	105.67 (6)
O15—Y9—O23^{viii}	80.64 (6)	Y7^{iii}—O20—Y14^{x}	129.43 (7)
O15—Y9—O22	78.25 (6)	Y7^{iii}—O20—Y11	104.78 (6)
O23^{viii}—Y9—O22	103.77 (6)	Y14^{x}—O20—Y11	104.63 (6)
O15—Y9—O25	177.52 (6)	Y7^{iii}—O20—Y14	104.94 (6)
O23^{viii}—Y9—O25	99.28 (6)	Y14^{x}—O20—Y14	98.81 (6)
O22—Y9—O25	99.39 (6)	Y11—O20—Y14	114.69 (7)
O15—Y9—O17	105.18 (6)	Y8^{iii}—O21—Y10	119.84 (7)
O23^{viii}—Y9—O17	85.86 (6)	Y8^{iii}—O21—Y7^{iii}	115.47 (7)
O22—Y9—O17	170.26 (6)	Y10—O21—Y7^{iii}	101.50 (6)
O25—Y9—O17	77.27 (6)	Y8^{iii}—O21—Y15	98.47 (6)
O15—Y9—O14	104.95 (6)	Y10—O21—Y15	117.68 (7)
O23^{viii}—Y9—O14	166.38 (6)	Y7^{iii}—O21—Y15	103.42 (6)
O22—Y9—O14	89.61 (6)	Y9—O22—Y8^{iii}	115.09 (7)
O25—Y9—O14	75.67 (6)	Y9—O22—Y16^{xi}	103.81 (6)
O17—Y9—O14	80.71 (6)	Y8^{iii}—O22—Y16^{xi}	101.78 (6)
O16—Y10—O26	77.73 (6)	Y9—O22—Y16	128.94 (7)
O16—Y10—O21	79.11 (6)	Y8^{iii}—O22—Y16	100.83 (6)
O26—Y10—O21	111.79 (6)	Y16^{xi}—O22—Y16	102.83 (6)
O16—Y10—O25	176.38 (6)	Y9^{ix}—O23—Y5	115.19 (7)
O26—Y10—O25	101.57 (6)	Y9^{ix}—O23—Y11	127.28 (7)
O21—Y10—O25	104.39 (6)	Y5—O23—Y11	100.19 (6)
O16—Y10—O14	105.23 (6)	Y9^{ix}—O23—Y13	101.97 (6)
O26—Y10—O14	163.87 (6)	Y5—O23—Y13	110.62 (7)
O21—Y10—O14	84.29 (6)	Y11—O23—Y13	100.31 (6)
O25—Y10—O14	74.45 (6)	Y12—O24—Y7	124.75 (8)
O16—Y10—O19	102.02 (6)	Y12—O24—Y15^{vi}	107.30 (7)
O26—Y10—O19	86.37 (6)	Y7—O24—Y15^{vi}	110.31 (7)
O21—Y10—O19	161.43 (6)	Y12—O24—Y14^{vi}	104.19 (6)
O25—Y10—O19	74.37 (5)	Y7—O24—Y14^{vi}	106.85 (6)
O14—Y10—O19	77.51 (6)	Y15^{vi}—O24—Y14^{vi}	100.67 (6)
O16—Y10—O31	123.07 (6)	Si4—O25—Y9	116.53 (8)

O26—Y10—O31	71.57 (6)	Si4—O25—Y12	114.63 (8)
O21—Y10—O31	69.97 (6)	Y9—O25—Y12	106.31 (6)
O25—Y10—O31	59.63 (5)	Si4—O25—Y10	105.81 (8)
O14—Y10—O31	117.33 (5)	Y9—O25—Y10	106.03 (6)
O19—Y10—O31	121.98 (6)	Y12—O25—Y10	106.82 (6)
O20—Y11—O16	75.89 (6)	Y10—O26—Y6^{ix}	112.77 (7)
O20—Y11—O28^{ix}	78.36 (6)	Y10—O26—Y13	125.02 (7)
O16—Y11—O28^{ix}	125.24 (6)	Y6^{ix}—O26—Y13	104.14 (7)
O20—Y11—O23	162.10 (6)	Y10—O26—Y11	102.55 (6)
O16—Y11—O23	122.00 (6)	Y6^{ix}—O26—Y11	108.66 (6)
O28^{ix}—Y11—O23	90.02 (6)	Y13—O26—Y11	102.45 (6)
O20—Y11—O9	113.46 (6)	Y16^{vi}—O27—Y15^{vi}	120.90 (7)
O16—Y11—O9	72.64 (6)	Y16^{vi}—O27—Y8	106.02 (7)
O28^{ix}—Y11—O9	74.83 (6)	Y15^{vi}—O27—Y8	101.61 (6)
O23—Y11—O9	75.75 (5)	Y16^{vi}—O27—Y13	106.97 (6)
O20—Y11—O26	109.58 (5)	Y15^{vi}—O27—Y13	109.56 (7)
O16—Y11—O26	71.68 (6)	Y8—O27—Y13	111.61 (7)
O28^{ix}—Y11—O26	163.06 (6)	Y12—O28—Y3^{vii}	126.58 (7)
O23—Y11—O26	78.39 (6)	Y12—O28—Y11^{viii}	124.62 (7)
O9—Y11—O26	113.44 (5)	Y3^{vii}—O28—Y11^{viii}	100.01 (6)
O20—Y11—O30	72.21 (6)	Y12—O28—Y14^{vi}	99.94 (6)
O16—Y11—O30	118.43 (6)	Y3^{vii}—O28—Y14^{vi}	100.67 (6)
O28^{ix}—Y11—O30	97.75 (6)	Y11^{viii}—O28—Y14^{vi}	98.62 (6)
O23—Y11—O30	96.28 (5)	Y4^{ix}—O29—Y12	119.57 (7)
O9—Y11—O30	168.90 (5)	Y4^{ix}—O29—Y13	102.27 (6)
O26—Y11—O30	71.65 (5)	Y12—O29—Y13	118.37 (7)
O24—Y12—O28	81.93 (6)	Y4^{ix}—O29—Y15^{vi}	113.01 (7)
O24—Y12—O29	78.96 (6)	Y12—O29—Y15^{vi}	100.15 (6)
O28—Y12—O29	105.13 (6)	Y13—O29—Y15^{vi}	102.53 (6)
O24—Y12—O25	177.11 (6)	Si3^{ix}—O30—Y6^{ix}	115.21 (9)
O28—Y12—O25	99.85 (6)	Si3^{ix}—O30—Y11	119.79 (9)
O29—Y12—O25	102.67 (6)	Y6^{ix}—O30—Y11	100.95 (6)
O24—Y12—O19	103.26 (6)	Si3^{ix}—O30—Y14	115.80 (8)
O28—Y12—O19	164.10 (6)	Y6^{ix}—O30—Y14	100.86 (6)
O29—Y12—O19	90.66 (6)	Y11—O30—Y14	101.37 (6)
O25—Y12—O19	74.42 (5)	Si4—O31—Y6^{ix}	124.64 (10)
O24—Y12—O17	102.60 (6)	Si4—O31—Y15	136.94 (10)
O28—Y12—O17	87.72 (6)	Y6^{ix}—O31—Y15	98.23 (6)
O29—Y12—O17	167.12 (6)	Si4—O31—Y10	88.42 (8)
O25—Y12—O17	75.27 (5)	Y6^{ix}—O31—Y10	91.53 (6)
O19—Y12—O17	76.51 (6)	Y15—O31—Y10	94.93 (7)
O27—Y13—O26	160.42 (6)	Si4—O31—Ba1^{xii}	67.62 (7)
O27—Y13—O15^{ix}	74.71 (6)	Y6^{ix}—O31—Ba1^{xii}	97.93 (6)
O26—Y13—O15^{ix}	124.66 (6)	Y15—O31—Ba1^{xii}	105.91 (6)
O27—Y13—O10^{ix}	118.30 (6)	Y10—O31—Ba1^{xii}	155.51 (7)
O26—Y13—O10^{ix}	74.01 (6)	Si4—O32—Y5^{viii}	129.38 (9)
O15^{ix}—Y13—O10^{ix}	74.47 (5)	Si4—O32—Y16	130.79 (9)
O27—Y13—O29	73.44 (6)	Y5^{viii}—O32—Y16	95.18 (6)

O26—Y13—O29	96.89 (6)	Si4—O32—Ba1^{xii}	80.42 (7)
O15^{ix}—Y13—O29	117.45 (6)	Y5^{viii}—O32—Ba1^{xii}	107.55 (6)
O10^{ix}—Y13—O29	75.62 (6)	Y16—O32—Ba1^{xii}	107.95 (6)
O27—Y13—O23	107.38 (5)	Y15—O33—Y6^{ix}	111.69 (7)
O26—Y13—O23	78.84 (5)	Y15—O33—Y1^{xii}	117.26 (7)
O15^{ix}—Y13—O23	72.93 (6)	Y6^{ix}—O33—Y1^{xii}	105.23 (7)
O10^{ix}—Y13—O23	112.50 (5)	Y15—O33—Y14	104.09 (6)
O29—Y13—O23	168.89 (6)	Y6^{ix}—O33—Y14	113.43 (7)
O27—Y13—O18	72.16 (6)	Y1^{xii}—O33—Y14	105.22 (6)
O26—Y13—O18	93.80 (6)		

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*−1, *y*, *z*; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*, *y*+1/2, −*z*+1/2; (v) −*x*, −*y*+1, −*z*+1; (vi) *x*, −*y*+1/2, *z*+1/2; (vii) −*x*+1, −*y*+1, −*z*+1; (viii) −*x*+1, *y*+1/2, −*z*+1/2; (ix) −*x*+1, *y*−1/2, −*z*+1/2; (x) −*x*+1, −*y*, −*z*; (xi) −*x*+1, −*y*+1, −*z*; (xii) *x*+1, *y*, *z*.