Supplementary Data

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

Shuto Motozawa,[1,2] Hiromitsu Kimura,[3] Junichi Takahashi,[1] Rayko Simura[1] and Hisanori Yamane[1*]

[1] Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Katahira 2-1-1 Aoba-ku, Sendai 980-8577, Japan

[2] 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

[3] Science & Innovation Center, Inorganic Materials Laboratory, Mitsubishi Chemical Corporation, 1000 Kamoshida-cho, Aoba-ku, Yokohama-shi, Kanagawa 227-8502, Japan
*Correspondence e-mail: hisanori.yamane.a1@tohoku.ac.jp

Fig. S1. Relative dielectric constant (ε_r) and dielectric loss (tan δ) of $BaY_{16}Si_4O_{33}$ ceramics at 298 K as functions of frequency (f).

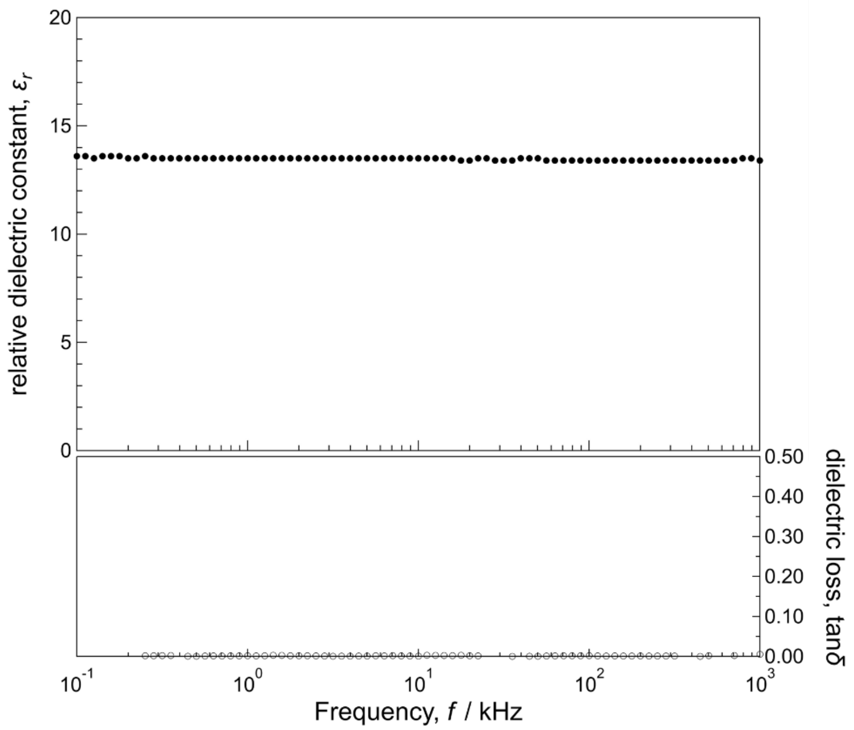
Fig. S2. Relative dielectric constant (ε_r) and dielectric loss (tan δ) of $BaY_{16}Si_4O_{33}$ ceramics at 1 MHz as function of temperature.

Fig. S3. Thermal expansion of $BaY_{16}Si_4O_{33}$ ceramic as function of temperature.

Fig. S4. Experimental (dot) and calculated (solid line) profiles obtained from Rietveld refinement of X-ray powder diffraction data for $BaY_{16}Si_4O_{33}$ at 298 K. The difference profile (bottom) is on the same scale. Vertical ticks indicate the calculated positions of all possible Bragg reflections for $BaY_{16}Si_4O_{33}$.

Table S1 Crystallographic data for $BaY_{16}Si_4O_{33}$, as derived from Rietveld refinement of powder XRD data.

Table S2 Atomic coordinates and overall isotropic displacement parameter (U_{iso}), as derived from Rietveld refinement of powder XRD data for $BaY_{16}Si_4O_{33}$.



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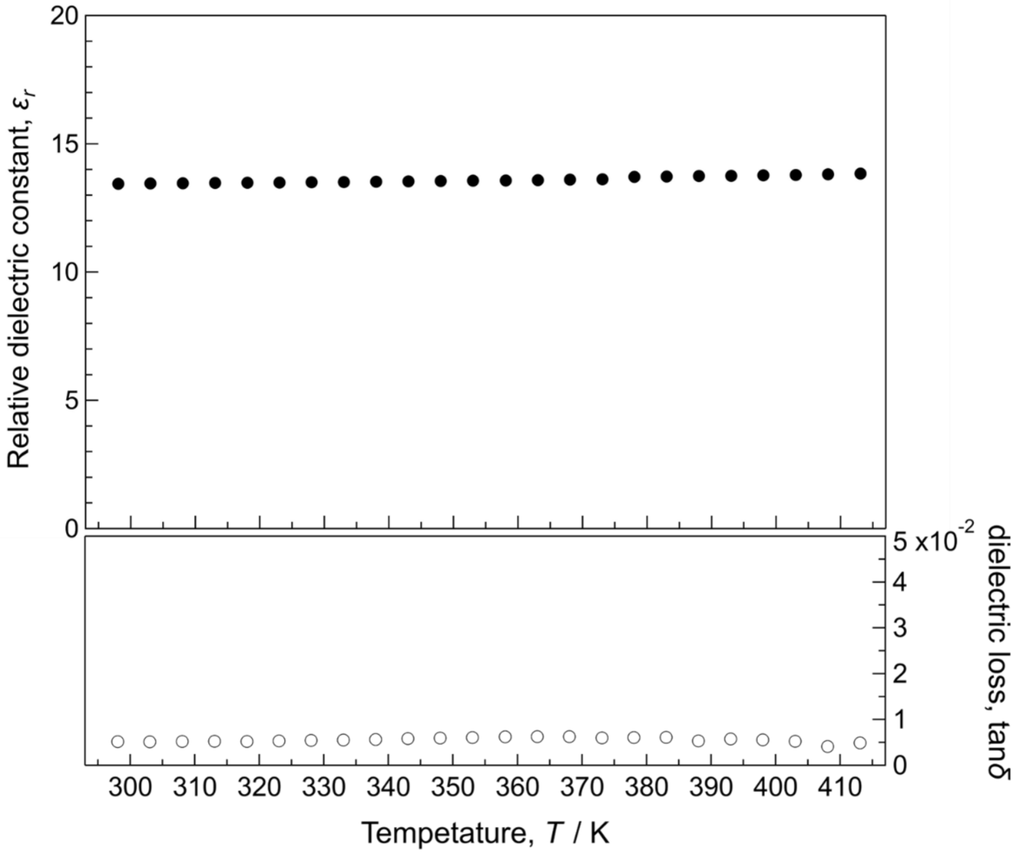

Fig. S2. Relative dielectric constant (ε_r) and dielectric loss (tan δ) of $BaY_{16}Si_4O_{33}$ ceramics at 1 MHz as function of temperature.

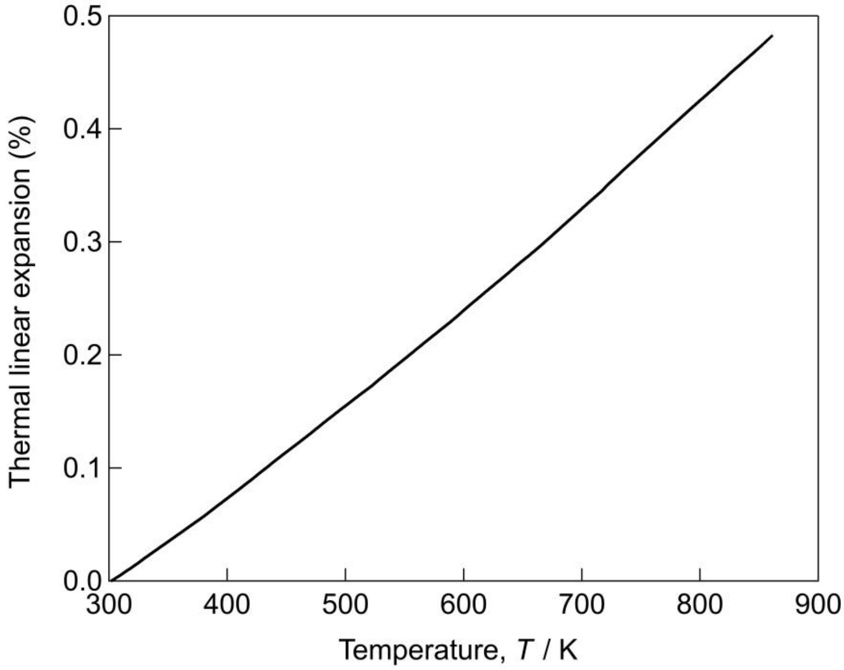

Fig. S3. Thermal expansion of $BaY_{16}Si_4O_{33}$ ceramic as function of temperature.

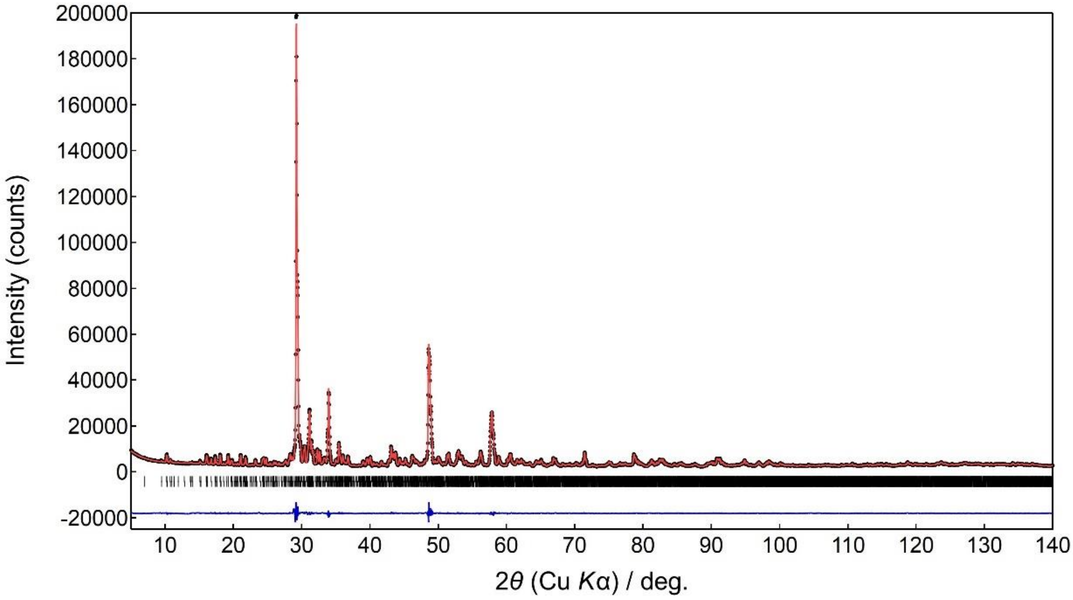

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Table S1 Crystallographic data for $BaY_{16}Si_4O_{33}$, as derived from Rietveld refinement of powder XRD data.

Chemical formula		$BaY_{16}Si_4O_{33}$
Temperature, T (K)		298(2)
Crystal system		monoclinic
Space group		$P12_1/c1$ (No.14)
Unit-cell dimensions	a (Å)	9.112340(80)
	b (Å)	18.73111(19)
	c (Å)	18.31827(17)
	β	109.04410(66)
Unit-cell volume, V (Å^3)		2955.511(49)
Z		4
Calculated density, D_{cal} (Mg m^{-3})		4.944526(82)
Radiation wavelength, λ (Å)		1.54059/1.54432
2θ range for date collection (°)		5.0 – 140.0
Reflections collected		5483
R_p , R_{wp}		0.0221, 0.0303
R_B		0.00752

$R_p = \Sigma|Y_{o,m} - Y_{c,m}|/\Sigma Y_{o,m}$, $R_{wp} = [\Sigma w_m(Y_{o,m}- Y_{c,m})^2/\Sigma w_m Y_{o,m}{}^2]^{1/2}$, $w_m = 1/\sigma(Y_{o,m})$, $R_B = \Sigma|I_{\text{"o"},k} - I_{c,k}|/\Sigma I_{\text{"o"},k}$, where $Y_{o,m}$ and $Y_{c,m}$ are the observed and calculated data, respectively at data point m; $\sigma(Y_{o,m})$ is the error in $Y_{o,m}$, and $I_{\text{"o"},k}$ and $I_{c,k}$ are the observed and calculated intensities of the kth reflection.

Table S2 Atomic coordinates and overall isotropic displacement parameter (U_{iso}), as derived from Rietveld refinement of powder XRD data for $BaY_{16}Si_4O_{33}$.

Atom	Wyckoff site	Occ.	*x*	*y*	*z*	U_{iso}
Ba1	4*e*	1	0.0518(4)	0.3484(3)	0.2131(2)	0.417(17)
Y1	4*e*	1	0.0269(7)	0.1413(4)	0.0850(3)	0.417
Y2	4*e*	1	0.0431(8)	0.5519(4)	0.1092(4)	0.417
Y3	4*e*	1	0.0655(8)	0.5470(4)	0.5884(4)	0.417
Y4	4*e*	1	0.0754(7)	0.7514(4)	0.1098(4)	0.417
Y5	4*e*	1	0.2156(7)	0.0312(3)	0.2848(4)	0.417
Y6	4*e*	1	0.2152(6)	0.6577(4)	0.3024(3)	0.417
Y7	4*e*	1	0.2859(7)	0.3462(5)	0.4711(3)	0.417
Y8	4*e*	1	0.3330(6)	0.1417(3)	0.4601(3)	0.417
Y9	4*e*	1	0.3940(8)	0.4480(4)	0.1514(4)	0.417
Y10	4*e*	1	0.3996(9)	0.2518(4)	0.1474(5)	0.417
Y11	4*e*	1	0.4054(8)	0.0583(4)	0.1499(4)	0.417
Y12	4*e*	1	0.5283(6)	0.3461(5)	0.3357(3)	0.417
Y13	4*e*	1	0.5941(7)	0.1375(4)	0.3391(4)	0.417
Y14	4*e*	1	0.6510(9)	0.0608(4)	0.0106(4)	0.417
Y15	4*e*	1	0.6560(9)	0.2475(4)	0.0109(4)	0.417
Y16	4*e*	1	0.6871(8)	0.4544(4)	0.0219(4)	0.417
Si1	4*e*	1	0.0504(19)	0.3464(14)	0.0466(10)	0.417
Si2	4*e*	1	0.200(2)	0.2139(10)	0.3000(12)	0.417
Si3	4*e*	1	0.212(2)	0.4819(10)	0.3066(11)	0.417
Si4	4*e*	1	0.7103(19)	0.3434(12)	0.2046(10)	0.417
O1	4*e*	1	0.028(4)	0.351(3)	0.4586(19)	0.417
O2	4*e*	1	0.031(4)	0.934(2)	0.434(2)	0.417
O3	4*e*	1	0.046(5)	0.1836(19)	0.225(2)	0.417
O4	4*e*	1	0.066(4)	0.784(2)	0.458(2)	0.417
O5	4*e*	1	0.064(5)	0.504(2)	0.233(2)	0.417
O6	4*e*	1	0.056(4)	0.144(3)	0.4557(19)	0.417
O7	4*e*	1	0.095(5)	0.552(2)	0.480(2)	0.417
O8	4*e*	1	0.150(5)	0.436(2)	0.366(2)	0.417
O9	4*e*	1	0.155(4)	0.043(2)	0.166(2)	0.417
O10	4*e*	1	0.168(4)	0.647(3)	0.1692(19)	0.417
O11	4*e*	1	0.164(4)	0.8317(19)	0.205(2)	0.417
O12	4*e*	1	0.158(5)	0.256(2)	0.360(2)	0.417
O13	4*e*	1	0.218(5)	0.048(2)	0.403(2)	0.417
O14	4*e*	1	0.217(4)	0.357(3)	0.0937(18)	0.417
O15	4*e*	1	0.266(5)	0.536(2)	0.099(3)	0.417

O16	4*e*	1	0.259(4)	0.155(3)	0.0943(19)	0.417
O17	4*e*	1	0.333(4)	0.433(2)	0.262(2)	0.417
O18	4*e*	1	0.301(4)	0.140(2)	0.3368(19)	0.417
O19	4*e*	1	0.310(5)	0.269(2)	0.258(2)	0.417
O20	4*e*	1	0.420(5)	0.062(2)	0.036(2)	0.417
O21	4*e*	1	0.411(5)	0.2612(18)	0.033(3)	0.417
O22	4*e*	1	0.442(5)	0.4548(19)	0.036(2)	0.417
O23	4*e*	1	0.446(5)	0.032(2)	0.287(2)	0.417
O24	4*e*	1	0.499(4)	0.342(2)	0.4392(18)	0.417
O25	4*e*	1	0.540(4)	0.345(3)	0.2046(19)	0.417
O26	4*e*	1	0.538(4)	0.163(2)	0.224(2)	0.417
O27	4*e*	1	0.565(4)	0.142(2)	0.4530(19)	0.417
O28	4*e*	1	0.660(5)	0.443(2)	0.387(2)	0.417
O29	4*e*	1	0.690(5)	0.250(2)	0.394(3)	0.417
O30	4*e*	1	0.664(5)	0.041(2)	0.147(2)	0.417
O31	4*e*	1	0.700(5)	0.270(2)	0.152(2)	0.417
O32	4*e*	1	0.748(4)	0.411(2)	0.162(2)	0.417
O33	4*e*	1	0.791(4)	0.164(2)	0.098(2)	0.417