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Supplementary Information

Thermal evolution of the $Ca_2B_2O_5$ crystal structure through γ ↔ β' ↔ α phase transitions and the crystal structure of the incommensurately modulated β' phase

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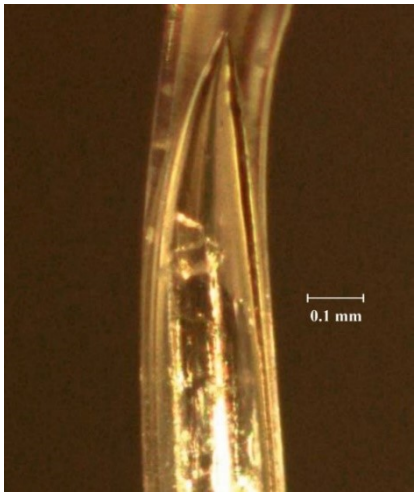

Figure S1 The photo of studied crystal of $Ca_2B_2O_5$.

Table S1 Phases of $Ca_2B_2O_5$ and $Sr_2B_2O_5$. T (K) are transition temperatures. Data on the mineral shimazakiite ($Ca_2B_2O_5$)[1] and its synthetic analogue[2] are not given in the table.

Ref.	[3]	[2]	[4], here	[5]	[6]
		$Ca_2B_2O_5$		$Sr_2B_2O_5$	
The low-temperature phase	β	α	γ	γ	γ
The intermediate phases	-	-	β' (784 K)	β (557 K), α' (634 K)	β (565 K), α' (637 K)
The high-temperature phase	α (804 K)	-	α (860 K)	α (646 K)	α (651 K)

Table S2 Experimental details for single–crystal X–ray diffraction studies of $Ca_2B_2O_5$ at 790 K.

Chemical formula	γ–$Ca_2B_2O_5$	β'–$Ca_2B_2O_5$
Temperature (K)	790	
Crystal data		
Crystal system	Monoclinic	
(Super)space group	$P2_1/c$	$P2_1/c(\alpha\beta\gamma)00(\alpha-\beta\gamma)00$
M_r	66.9	181.8
a (Å)	3.6351(9)	3.632(1)
b (Å)	5.2092(7)	5.207(2)
c (Å)	11.620(4)	11.638(2)

α (°)	90	90
β (°)	92.35(3)	92.31(2)
γ (°)	90	90
V (Å^3)	219.9(1)	219.92(4)
Z	4	2
μ (mm^{-1})	2.42	2.51
Modulation wavevectors	$\mathbf{q}$=0.5$\mathbf{a}^*$	$\mathbf{q_1}$=–0.141(3)$\mathbf{a}^*$+ 0.381(4)$\mathbf{b}^*$+ 0.110(1)$\mathbf{c}^*$
	–	$\mathbf{q_2}$=–0.141(3)$\mathbf{a}^*$–0.381(4)$\mathbf{b}^*$+ 0.110(1)$\mathbf{c}^*$
Crystal form	Prism	
Crystal size (mm^3)	0.052 × 0.109 × 0.124	
Color	Colorless	
Data collection		
Diffractometer	XtaLAB Synergy	
Radiation type	Mo *K*a	
Wavelength	0.71073	
Diffractometer	Multi–scan *CrysAlis PRO* 1.171.42.49 (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	
Indexes ranges	–5 ≤ h ≤ 5 –6 ≤ k ≤ 4 –15 ≤ l ≤ 15 –1 ≤ m ≤ 1	–4 ≤ h ≤ 4 –7 ≤ k ≤ 5 –15 ≤ l ≤ 15 –1 ≤ m ≤ 1 –1 ≤ n ≤ 1
No. of measured reflections	4190	11391
No. of unique reflections	1065	2673
No. of observed reflections	425	788
No. of main reflections	531	532
No. of observed first–order satellites	534	2141
R_{int} (all reflections)	0.079	0.100
R_{int} (main reflections)	0.077	0.060
$R_{int,all}$, $R_{int,obs}$ (first–order satellites)	0.082, 0.075	0.493, 0.274
Refinement		
R_{all}, wR_{all}	0.260, 0.135	0.193, 0.165
R_{obs}, wR_{obs}	0.092, 0.121	0.070, 0.140
R_{obs}, R_{all}, wR_{all} (main reflections)	0.073, 0.099, 0.089	0.056, 0.078, 0.131
R_{obs}, R_{all}, wR_{all} (first–order satellites)	0.497, 1.659, 0.498	0.107, 0.345, 0.263
S_{obs}, S_{all}	5.05, 3.32	2.36, 1.38
No. of parameters	82	218
Δp_{max} (e Å^{-3})	2.84	1.73
Δp_{min} (e Å^{-3})	–2.18	–1.42

Computer programs used: *CrysAlis PRO* 1.171.42.49 (Rigaku Oxford Diffraction, 2022), *Jana2020* (Petříček et al., 2023).

Table S3 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 300 K.

Atom	SOF	x	y	z	U_{eq}
Ca1	1	0.7583(1)	–0.41713(8)	0.14859(3)	0.0085(1)
O1	0.5	0.7832(5)	0.8065(3)	0.3581(2)	0.0106(6)
O1'	0.5	0.7122(5)	0.8215(3)	0.4292(2)	0.0101(6)
O2	1	0.7622(4)	0.3878(3)	0.3339(1)	0.0107(4)
O3	0.5	0.4549(5)	0.0923(3)	–0.0160(2)	0.0127(6)
B1	1	0.6818(6)	0.5696(4)	0.4075(2)	0.0086(6)

Table S4 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 300 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0085(2)	0.0081(2)	0.0089(2)	0.0001(1)	0.0014(2)	0.0008(1)
O1	0.009(1)	0.008(1)	0.014(1)	0	0.0037(8)	0.0014(7)
O1'	0.013(1)	0.0063(9)	0.010(1)	0	0	0
O2	0.0127(7)	0.0100(7)	0.0095(7)	0.0026(5)	0.0023(6)	0
O3	0.018(1)	0.010 (1)	0.0111(1)	0.0047(8)	0.0065(8)	0.0021(8)
B1	0.007(1)	0.010(1)	0.009 (1)	0.0016(8)	0	0.0013(8)

Table S5 Displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 300 K.

Atom	Wave	*x*	*y*	*z*
Ca1	s,1	0.0078(2)	–0.0259(1)	–0.02252(5)
O2	o,1	–0.1097(7)	–0.0655(5)	0.0177(2)
B1	s,1	–0.0094(7)	–0.0082(4)	0.0042(2)

Table S6 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 300 K.

Atom		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1	–0.0001(3)	0.0008(3)	–0.0006(3)	0.0001(2)	0.0008(2)	0.0003(2)
O2	o,1	–0.006(1)	–0.005(1)	0.004(1)	–0.005(1)	–0.001(1)	–0.000 (1)
B1	s,1	0.001(1)	0.002(1)	–0.003(1)	–0.0007(9)	–0.001(1)	0.003(1)

Table S7 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 300 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.474 (2)	2.474(2)	2.474(2)
Ca1–O1(ii)	2.394(3)	2.394(3)	2.394(3)
Ca1–O1(iii)	2.291(3)	2.291(3)	2.291(3)
Ca1–O1'(ii)	2.427(2)	2.427(2)	2.427(2)
Ca1– O1'(iii)	2.415(3)	2.415(3)	2.415(3)
Ca1– O1'(iv)	2.419(2)	2.419(2)	2.419(2)
Ca1–O2(i)	2.385(2)	2.335(2)	2.435(2)
Ca1–O2(v)	2.474(3)	2.297(3)	2.651(3)
Ca1–O2(vi)	2.389(3)	2.359(3)	2.419(3)
Ca1–O3(vii)	2.427(2)	2.427(2)	2.427(2)
B1–O1	1.354(3)	1.354(3)	1.354(3)
B1–O1'	1.364(3)	1.364(3)	1.364(3)
B1–O2	1.354(3)	1.350(3)	1.357(3)
B1–O3(viii)	1.416(3)	1.416(3)	1.416(3)
B1–O3(ix)	1.434(3)	1.434(3)	1.434(3)

Symmetry codes: (i) x, y–1, z; (ii) –x+1, y–3/2, –z+1/2; (iii) –x+2, y–3/2, –z+1/2; (iv) x, –y+1/2, z–1/2; (v) –x+1, y–1/2, –z+1/2; (vi) –x+2, y–1/2, –z+1/2; (vii) –x+1, –y, –z; (viii) –x+1, y+1/2, –z+1/2; (ix) x, –y+1/2, z+1/2.

Table S8 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 500 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7600(1)	-0.41641(7)	0.14824(3)	0.0139(1)
O1	0.5	0.7816(5)	0.8074(3)	0.3593 (2)	0.0188(6)
O1'	0.5	0.7125(5)	0.8223(3)	0.4290(2)	0.0150(6)
O2	1	0.7617(4)	0.3889(2)	0.3339(1)	0.0175(4)
O3	0.5	0.4567(5)	0.0897(3)	-0.0157(2)	0.0220(6)
B1	1	0.6819(6)	0.5708(4)	0.4076(2)	0.0128(6)

Table S9 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 500 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0140(2)	0.0129(2)	0.0151(2)	0.00073(14)	0.0019(2)	0.0012(1)
O1	0.021(1)	0.012(1)	0.025 (1)	0	0.0064(9)	0.0040(7)
O1'	0.017(1)	0.0113(9)	0.017(1)	0	0.0006(8)	0
O2	0.0217(8)	0.0164(7)	0.0149(7)	0.0034(5)	0.0046(6)	0
O3	0.034(1)	0.016 (1)	0.017 (1)	0.0097(8)	0.0103(9)	0.0040(8)
B1	0.0095(9)	0.015(1)	0.014(1)	0.0002(8)	0	0.0018(8)

Table S10 Displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 500 K.

Atom	Wave	*x*	*y*	*z*
Ca1	s,1	0.0071(1)	–0.02513(9)	–0.02165(5)
O2	o,1	–0.1078(7)	–0.0645(4)	0.0172(2)
B1	s,1	–0.0093(6)	–0.0070(4)	0.0041(2)

Table S11 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 500 K.

Atom		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1	–0.0003(3)	0.0020(3)	–0.0014(3)	0.0004(2)	0.0019(2)	0.0003(2)
O2	o, 1	–0.008(1)	–0.007(1)	0.004(1)	–0.0081(1)	–0.001(1)	–0.002(1)
B1	s,1	0.002(1)	0.001(1)	–0.004(1)	0.0004(9)	–0.003(1)	0.0010(1)

Table S12 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 500 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.501(2)	2.501(2)	2.501(2)
Ca1–O1(ii)	2.401(4)	2.401(4)	2.401(4)
Ca1–O1(iii)	2.293(3)	2.293(3)	2.293(3)
Ca1–O1' (ii)	2.433(3)	2.433(3)	2.433(3)
Ca1– O1'(iii)	2.420(3)	2.420(3)	2.420(3)
Ca1– O1'(iv)	2.425(2)	2.425(2)	2.425(2)
Ca1–O2(i)	2.388(2)	2.337(2)	2.440(2)
Ca1–O2(v)	2.487(3)	2.310(3)	2.664(3)
Ca1–O2(vi)	2.392(3)	2.362(3)	2.422(3)
Ca1–O3(vii)	2.436(2)	2.436(2)	2.436(2)
B1–O1	1.353(3)	1.353(3)	1.353(3)
B1–O1'	1.359(3)	1.359(3)	1.359(3)
B1–O2	1.354(3)	1.349(3)	1.359(3)
B1–O3(viii)	1.416(3)	1.416(3)	1.416(3)
B1–O3(ix)	1.430(3)	1.430(3)	1.430(3)

Symmetry codes: (i) x, y–1, z; (ii) –x+1, y–3/2, –z+1/2; (iii) –x+2, y–3/2, –z+1/2; (iv) x, –y+1/2, z–1/2; (v) –x+1, y–1/2, –z+1/2; (vi) –x+2, y–1/2, –z+1/2; (vii) –x+1, –y, –z; (viii) –x+1, y+1/2, –z+1/2; (ix) x, –y+1/2, z+1/2.

Table S13 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 700 K.

Atom	SOF	x	y	z	U_{eq}
Ca1	1	0.7614(1)	–0.4149 (1)	0.14775(4)	0.0199(1)
O1	0.5	0.7797(6)	0.8088(4)	0.3612(2)	0.0276(8)
O1'	0.5	0.7126(6)	0.8227(4)	0.4284(1)	0.0212(8)
O2	1	0.7601(5)	0.3916(3)	0.3336(1)	0.0255(6)
O3	0.5	0.4570(7)	0.0865(4)	–0.0157(2)	0.0325(9)
B1	1	0.6810(7)	0.5722(6)	0.4076(2)	0.0188(8)

Table S14 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 700 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0190(3)	0.0189(3)	0.0219(3)	0.0007(2)	0.0035(2)	0.0019(2)
O1	0.027(1)	0.015(1)	0.041(2)	0	0.011(1)	0.006(1)
O1'	0.026(1)	0.015(1)	0.024(1)	0	0.003(1)	0.0004(9)
O2	0.031(1)	0.024(1)	0.0220(9)	0.0054(8)	0.0074(8)	0)
O3	0.048(2)	0.026 (2)	0.025(1)	0.014(1)	0.017(1)	0.007(1)
B1	0.016(1)	0.022(2)	0.019(1)	0	0.001(1)	0.002(1)

Table S15 Displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 700 K.

Atom	Wave	x	y	z
Ca1	s,1	0.0063 (2)	–0.0238(1)	–0.02035(6)
O2	o,1	–0.1067(9)	–0.0636(6)	0.0160(3)
B1	s,1	–0.0088(8)	–0.0066(6)	0.0043(3)

Table S16 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 700 K.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1	–0.0007(4)	0.0028(4)	–0.0034(4)	0.0007(3)	0.0025(3)	0.0003(3)
O2	o,1	–0.012(2)	–0.009(2)	0.008(2)	–0.010(2)	–0.001(2)	–0.003(1)
B1	s,1	–0.001(2)	0.003(2)	–0.002(2)	0.002(1)	–0.003(1)	–0.002(1)

Table S17 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 700 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.542(2)	2.542(2)	2.542(2)
Ca1–O1(ii)	2.407(4)	2.407(4)	2.407(4)
Ca1–O1(iii)	2.296(3)	2.296(3)	2.296(3)
Ca1–O1' (ii)	2.439(3)	2.439(3)	2.439(3)
Ca1– O1'(iii)	2.428(4)	2.428(4)	2.428(4)
Ca1– O1'(iv)	2.436(2)	2.436(2)	2.436(2)
Ca1–O2(i)	2.389(2)	2.337(2)	2.442(2)
Ca1–O2(v)	2.499(4)	2.319(4)	2.679(4)
Ca1–O2(vi)	2.402(3)	2.373(4)	2.430(4)
Ca1–O3(vii)	2.442(2)	2.442(2)	2.442(2)
B1–O1	2.499(4)	2.319(4)	2.679(4)
B1–O1'	2.402(3)	2.373(4)	2.430(4)
B1–O2	2.442(2)	2.442(2)	2.442(2)
B1–O3(viii)	1.347(4)	1.347(4)	1.347(4)
B1–O3(ix)	1.353(4)	1.353(4)	1.353(4)

Symmetry codes: (i) x, y–1, z; (ii) –x+1, y–3/2, –z+1/2; (iii) –x+2, y–3/2, –z+1/2; (iv) x, –y+1/2, z–1/2; (v) –x+1, y–1/2, –z+1/2; (vi) –x+2, y–1/2, –z+1/2; (vii) –x+1, –y, –z; (viii) –x+1, y+1/2, –z+1/2; (ix) x, –y+1/2, z+1/2.

Table S18 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 750 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7618(1)	–0.4138(1)	0.14746(4)	0.0216(2)
O1	0.5	0.7800(6)	0.8102(5)	0.3621(2)	0.0310(8)
O1'	0.5	0.7147(6)	0.8246(4)	0.4284(2)	0.0236(8)
O2	1	0.7600(5)	0.3929(3)	0.3332(1)	0.0273(6)
O3	0.5	0.4569(7)	0.0855(5)	–0.0157 (2)	0.0356(9)
B1	1	0.6816(7)	0.5739(6)	0.4080(2)	0.0192(8)

Table S19 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 750 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0217(3)	0.0197(3)	0.0236(3)	0.0009(2)	0.0039(2)	0.0022(2)
O1	0.029(14	0.017(2)	0.048(2)	0	0.011(1)	0.008(1)
O1'	0.029(1)	0.016(1)	0.027(1)	0	0.003(1)	0
O2	0.036(1)	0.023(1)	0.0245(9)	0.0055(8)	0.0087(8)	0
O3	0.053(2)	0.029(2)	0.026(1)	0.015(1)	0.019(1)	0.007(1)
B1	0.018(1)	0.019(2)	0.020(1)	0.002(1)	0.001(1)	0.002(1)

Table S20 Displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 750 K.

Atom	Wave	*x*	*y*	*z*
Ca1	s,1	0.0062(2)	–0.0230(1)	–0.01972(6)
O2	o,1	–0.1041(9)	–0.0627(6)	0.0158(2)
B1	s,1	–0.0082(8)	–0.0047(6)	0.0039(2)

Table S21 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 750 K.

Atom		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1	0.0001(4)	0.0031(4)	–0.0045(4)	0.0004(3)	0.0027(3)	0.0002(3)
O2	o,1	–0.014(2)	–0.006(2)	0.009(2)	–0.012(2)	0.001(2)	–0.004(1)
B1	s,1	0.002(2)	0.001(2)	–0.004(1)	0.001(1)	–0.001(1)	–0.000(1)

Table S22 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 750 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.560(2)	2.560(2)	2.560(2)
Ca1–O1(ii)	2.411(4)	2.411(4)	2.411(4)
Ca1–O1(iii)	2.294(3)	2.294(3)	2.294(3)
Ca1–O1' (ii)	2.440(3)	2.440(3)	2.440(3)
Ca1– O1'(iii)	2.423(4)	2.423(4)	2.423(4)
Ca1– O1'(iv)	2.433(2)	2.433(2)	2.433(2)
Ca1–O2(i)	2.386(2)	2.332(2)	2.440(2)

Ca1–O2(v)	2.504(4)	2.327(4)	2.682(4)
Ca1–O2(vi)	2.403(3)	2.374(4)	2.432(4)
Ca1–O3(vii)	2.438(2)	2.438(2)	2.438(2)
B1–O1	2.504(4)	2.327(4)	2.682(4)
B1–O1'	2.403(3)	2.374(4)	2.432(4)
B1–O2	2.438(2)	2.438(2)	2.438(2)
B1–O3(viii)	1.353(4)	1.353(4)	1.353(4)
B1–O3(ix)	1.347(4)	1.347(4)	1.347(4)

Symmetry codes: (i) x, y–1, z; (ii) –x+1, y–3/2, –z+1/2; (iii) –x+2, y–3/2, –z+1/2; (iv) x, –y+1/2, z–1/2; (v) –x+1, y–1/2, –z+1/2; (vi) –x+2, y–1/2, –z+1/2; (vii) –x+1, –y, –z; (viii) –x+1, y+1/2, –z+1/2; (ix) x, –y+1/2, z+1/2.

Table S23 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 770 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7622(1)	–0.41324(8)	0.14738(4)	0.0219 (1)
O1	0.5	0.7794(5)	0.8104(4)	0.3626(2)	0.0320(7)
O1'	0.5	0.7146(5)	0.8242(3)	0.4283(2)	0.0250(6)
O2	1	0.7598(4)	0.3935(3)	0.3331(1)	0.0284(5)
O3	0.5	0.4568(6)	0.0846(4)	–0.0156(2)	0.0368(8)
B1	1	0.6814(6)	0.5733(4)	0.4079(2)	0.0194(7)

Table S24 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 770 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0210(2)	0.0204(3)	0.0246(2)	0.0009(2)	0.0025(2)	0.0024(2)
O1	0.029(1)	0.019(1)	0.048(1)	0	0.009(1)	0.0093(9)
O1'	0.029(1)	0.017(1)	0.029(1)	0	0.0009(9)	0
O2	0.0353(9)	0.0255(8)	0.0250(9)	0.0056(6)	0.0073(7)	0
O3	0.052(2)	0.031(1)	0.029(1)	0.016(1)	0.018(1)	0.0073(9)
B1	0.018(1)	0.019(1)	0.021(1)	0.0016(9)	0.0002(9)	0.0013(9)

Table S25 Displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 770 K.

Atom	Wave	*x*	*y*	*z*
Ca1	s,1	0.00611(15)	–0.02246(10)	–0.01939(5)
O2	o,1	–0.1029(7)	–0.0616(5)	0.0156(2)
B1	s,1	–0.0087(7)	–0.0059(4)	0.0036(2)

Table S26 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 770 K.

Atom		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1	–0.0003(3)	0.0035(3)	–0.0048(3)	0.0004(2)	0.0027(3)	–0.0002(2)
O2	o,1	–0.014 (2)	–0.009(2)	0.009(2)	–0.011(1)	–0.002(1)	–0.004(1)
B1	s,1	0.002(1)	0.0025(13)	–0.005(1)	0.000(1)	–0.003(1)	0.000(1)

Table S27 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 770 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.569(2)	2.569(2)	2.569(2)
Ca1–O1(ii)	2.413(3)	2.413(3)	2.413(3)
Ca1–O1(iii)	2.295(3)	2.295(3)	2.295(3)
Ca1–O1' (ii)	2.442(3)	2.442(3)	2.442(3)
Ca1– O1'(iii)	2.427(3)	2.427(3)	2.427(3)
Ca1– O1'(iv)	2.437(2)	2.437(2)	2.437(2)
Ca1–O2(i)	2.386(2)	2.333(2)	2.439(2)
Ca1–O2(v)	2.506(3)	2.330(3)	2.682(3)
Ca1–O2(vi)	2.402(3)	2.375(3)	2.430(3)
Ca1–O3(vii)	2.440(2)	2.440(2)	2.440(2)
B1–O1	2.506(3)	2.330(3)	2.682(3)
B1–O1'	2.402(3)	2.375(3)	2.430(3)
B1–O2	2.440(2)	2.440(2)	2.440(2)
B1–O3(viii)	1.350(3)	1.350(3)	1.350(3)
B1–O3(ix)	1.354(3)	1.354(3)	1.354(3)

Symmetry codes: (i) x, y–1, z; (ii) –x+1, y–3/2, –z+1/2; (iii) –x+2, y–3/2, –z+1/2; (iv) x, –y+1/2, z–1/2; (v) –x+1, y–1/2, –z+1/2; (vi) –x+2, y–1/2, –z+1/2; (vii) –x+1, –y, –z; (viii) –x+1, y+1/2, –z+1/2; (ix) x, –y+1/2, z+1/2.

Table S28 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 810 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7643(1)	–0.4018(1)	0.14440(5)	0.0299(2)
O1	1	0.7493(5)	0.8257(4)	0.4010(2)	0.0580(9)
O2	1	0.7492(6)	0.4056(3)	0.3298(2)	0.0416(8)
O3	0.5	0.477(1)	0.0812(5)	–0.0138(3)	0.044(1)
B1	1	0.6782(8)	0.5822(5)	0.4080(2)	0.0216(8)

Table S29 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 810 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0216(3)	0.0233(3)	0.0447(4)	0	0.0014(2)	0.0087(2)
O1	0.034(1)	0.023(1)	0.116(2)	0	0	0.001(1)
O2	0.049(2)	0.038(1)	0.038(1)	0.0129(9)	0.002(1)	0
O3	0.066(3)	0.037(2)	0.033(2)	0.013(2)	0.024(2)	0.010(1)
B1	0.019(1)	0.022(1)	0.023(1)	0.002(1)	0	0

Table S30 Displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 810 K.

Atom	SOF	Wave	*x*	*y*	*z*
Ca1	1	s,1,0	–0.0046(2)	0.0054(1)	0.00551(6)
	1	c,1,0	–0.0058(2)	0.0099(1)	0.00656(6)
	1	s,0,1	–0.00292(19)	0.0047(1)	0.01132(6)
	1	c,0,1	0.0014(2)	0.0005(1)	0.00593(6)
O1	1	s,1,0	–0.0069(7)	–0.0037(4)	0.0111(3)
	1	c,1,0	0.0012(8)	0.0010(4)	–0.0024(3)
	1	s,0,1	0.0112(7)	–0.0019(4)	–0.0158(3)
	1	c,0,1	0.0142(7)	0.0095(4)	–0.0231(3)
O2	1	s,1,0	–0.0151(7)	–0.0007(4)	0.0009(2)
	1	c,1,0	–0.0024(7)	0.0034(4)	0.0049(2)
	1	s,0,1	–0.0250(7)	–0.0215(4)	0.0135(2)
	1	c,0,1	–0.0037(7)	0.0061(4)	0.0006(2)
O3	0.5	s,1,0	–0.0101	–0.0077	–0.0014
	0.5	c,1,0	0.0155	–0.0017	0
	0.5	s,0,1	–0.0183	0.0035	0.0063
	0.5	c,0,1	–0.0104	0.0135	–0.0008
B1	1	s,1,0	–0.012(1)	–0.0045(7)	0.0070(3)
	1	c,1,0	0.002(1)	0.0007(7)	0.0030(3)
	1	s,0,1	–0.001(1)	0.0090(7)	–0.0007(3)
	1	c,0,1	0.001(1)	0.0094(7)	–0.0003(3)

Table S31 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 810 K.

Atom		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1,0	–0.0016(5)	–0.0012(4)	0.0057(5)	0.0008(3)	–0.0003(3)	0.0005(3)
	c,1,0	–0.0002(5)	–0.0015(4)	0.0117(5)	0.0015(3)	0.0000(3)	0.0039(3)
	s,0,1	–0.0010(5)	–0.0016(4)	–0.0030(5)	0.0006(3)	–0.0001(3)	–0.0004(3)
	c,0,1	0.0001(4)	0.0024(4)	0.0124(5)	–0.0006(3)	–0.0016(3)	0.0051(3)
O1	s,1,0	–0.001(2)	–0.001(2)	0.020(3)	0.000(1)	–0.0042(19)	–0.000(2)
	c,1,0	0.001(2)	–0.002(1)	0.076(3)	0.000(1)	–0.0150(19)	–0.001(2)
O2	s,1,0	–0.008(2)	–0.007(2)	–0.001(2)	–0.009(1)	0.0044(13)	0.003(1)
	c,1,0	0.006(2)	0.006(2)	0.006(2)	0.007(1)	–0.0020(13)	–0.005(1)
	s,0,1	–0.005(2)	–0.000(2)	0.006(2)	–0.002(1)	–0.0025(13)	–0.003(1)
	c,0,1	0.008(2)	0.005(2)	0.007(2)	0.005(1)	–0.0029(13)	–0.005(1)
O3	s,1,0	–0.01245	–0.01453	–0.00026	0.000573	–0.00182	0.005036
	c,1,0	0.00573	–0.00111	–0.00048	0.003248	–0.00288	–0.00607
	s,0,1	0.001299	–0.00411	–0.00516	–0.0011	–0.00084	–0.00135
	c,0,1	–0.00154	–0.00023	0.001883	0.000008	–0.00189	0.005508
B1	s,1,0	0.001(2)	0.001(2)	–0.001(2)	0.001(2)	–0.002(2)	0.001(2)
	c,1,0	0.001(2)	–0.002(2)	0.001(2)	0.003(2)	–0.002(2)	–0.001(2)

s,0,1	–0.003(2)	–0.003(2)	0.002(2)	0.000(2)	0.002(2)	0.000(2)
c,0,1	–0.002(2)	0.002(2)	0.000(2)	–0.001(2)	–0.001(2)	–0.000(2)

Table S32 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 810 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.400(6)	2.360(6)	2.459(6)
Ca1–O1(ii)	2.352(6)	2.268(6)	2.438(6)
Ca1–O1(iii)	2.854(7)	2.321(7)	3.406(7)
Ca1–O2(iv)	2.387(5)	2.290(5)	2.473(5)
Ca1–O2(v)	2.490(5)	2.372(5)	2.615(5)
Ca1–O2(vi)	2.403(5)	2.350(5)	2.442(5)
Ca1–O3(vii)	2.405(3)	2.371(3)	2.437(3)
B1–O1	1.318(9)	1.280(9)	1.363(9)
B1–O2	1.341(9)	1.303(9)	1.387(9)
B1–O3(viii)	1.375(8)	1.334(8)	1.426(8)
B1–O3(ix)	1.464(8)	1.402(8)	1.534(8)

Symmetry codes: (i) *–x+1, y–3/2, –z+1/2*; (ii) *–x+2, y–3/2, –z+1/2*; (iii) *x, –y+1/2, z–1/2*; (iv) *x, y–1, z*; (v) *–x+1, y–1/2, –z+1/2*; (vi) *–x+2, y–1/2, –z+1/2*; (vii) *–x+1, –y, –z*; (viii) *–x+1, y+1/2, –z+1/2*; (ix) *x, –y+1/2, z+1/2*.

Table S33 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the supercell structure of $Ca_2B_2O_5$ at 810 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.4786(2)	0.2259(1)	0.8279(1)	0.027(1)
Ca2	1	0.0354(2)	-0.1037(1)	0.9039(1)	0.0154(9)
Ca3	1	0.5125(2)	0.0969(1)	0.6697(1)	0.027(1)
Ca4	1	0.5714(2)	0.5250(1)	1.2075(1)	0.026(1)
Ca5	1	0.8124(2)	0.6534 (1)	0.6506(1)	0.028(1)
Ca6	1	0.6572(2)	0.0971(1)	0.8124(1)	0.031(1)
Ca7	1	0.1547(2)	0.1491(1)	1.0094(1)	0.026(1)
Ca8	1	0.0483(2)	0.0260(1)	0.7118(1)	0.025(1)
Ca9	1	0.2999 (2)	0.1488(1)	1.1522(1)	0.0178(9)
Ca10	1	0.3774(2)	0.1005(1)	0.5265(1)	0.024(1)
Ca11	1	0.2648(2)	-0.2768(1)	0.6111(1)	0.026(1)
Ca12	1	0.6454(2)	0.3524(1)	0.7739(1)	0.0194(9)
Ca13	1	0.2023(2)	0.0248(1)	0.8535(1)	0.028(1)
Ca14	1	0.8934(2)	-0.1033(1)	0.7625(1)	0.031(1)
Ca15	1	0.0397(2)	0.2715(1)	0.6672(1)	0.025(1)
Ca16	1	0.1836(2)	0.2715(1)	0.8086(1)	0.023(1)
Ca17	1	0.8966(2)	0.2244(1)	1.2568(1)	0.033(1)
Ca18	1	0.0379(2)	0.2243(1)	0.3989(1)	0.024(1)
Ca19	1	0.4969(2)	0.3523 (1)	0.6334(1)	0.033(1)
Ca20	1	0.6797(2)	0.3987(1)	0.5472(1)	0.027(1)
Ca21	1	0.7880(2)	0.3538(1)	0.9158(1)	0.026(1)
Ca22	1	-0.0890(2)	0.0278(1)	0.5701(1)	0.026 (1)
Ca23	1	0.6480(2)	-0.0228(1)	1.0082(1)	0.032(1)
Ca24	1	0.1838(2)	0.2257(1)	0.5424(1)	0.0171(9)
Ca25	1	0.7243(2)	0.4727(1)	1.0759(1)	0.026(1)
Ca26	1	0.4962(2)	-0.0215(1)	0.8673(1)	0.0173(9)
Ca27	1	0.8142(2)	0.1001(1)	0.9541(1)	0.029(1)
Ca28	1	1.0471(3)	0.3475(1)	1.2075(1)	0.031(1)
Ca29	1	0.8726(2)	0.4756(1)	1.2199(1)	0.027(1)
Ca30	1	0.8285(2)	0.3969(1)	0.6883(1)	0.023(1)
Ca31	1	0.5767(2)	0.4735(1)	0.9331(1)	0.027(1)
Ca32	1	0.5845(3)	0.2776(1)	1.2485(1)	0.037(1)
Ca33	1	1.0207(2)	0.6022(1)	1.1695(1)	0.025(1)
Ca34	1	0.2715(3)	0.4026(1)	1.1148(1)	0.038(1)
Ca35	1	0.5598(3)	-0.1474(1)	0.7039(1)	0.035(1)
Ca36	1	0.4190(2)	-0.1484(1)	0.5626(1)	0.025(1)
Ca37	1	1.0123(2)	0.4765(1)	1.3656(1)	0.024(1)
Ca38	1	0.7261(2)	0.1509(1)	0.5827(1)	0.031(1)
Ca39	1	0.4614(2)	0.6019(1)	0.5983(1)	0.034(1)
Ca40	1	0.3174(2)	0.2727(1)	0.9553(1)	0.033(1)
Ca41	1	0.6205(2)	0.2239(1)	0.9689(1)	0.027(1)
Ca42	1	0.8672(2)	0.1512(1)	0.7243(1)	0.022(1)

Ca43	1	0.0101(2)	0.1519(1)	0.8681(1)	0.027(1)
Ca44	1	-0.1136(2)	0.2757(1)	0.5293(1)	0.0194(9)
Ca45	1	0.3406(3)	0.3499(1)	0.4929(1)	0.031(1)
Ca46	1	0.4484(2)	0.2749(1)	1.1015(2)	0.042(2)
Ca47	1	0.2437(3)	0.1023(1)	0.3823(1)	0.039(1)
Ca48	1	0.7549(3)	0.2244(1)	1.1133(1)	0.036(1)
Ca49	1	0.1497(2)	0.4775(1)	0.5085(1)	0.028(1)
Ca50	1	0.3342(2)	0.2267(1)	0.6852 (1)	0.024(1)
Ca51	1	0.5896(3)	0.5977(1)	0.7404(1)	0.042(1)
Ca52	1	0.2890(2)	0.4772(1)	0.6520(1)	0.029(1)
Ca53	1	1.1293(2)	0.4009(1)	0.9729(1)	0.022(1)
Ca54	1	0.2207(3)	-0.0258(1)	0.5766(1)	0.045(1)
Ca55	1	0.3541(2)	-0.0235(1)	0.7247(1)	0.031(1)
Ca56	1	0.9162(3)	0.3498(1)	1.0605(1)	0.049(2)
O1	1	0.7476(1)	0.5169(4)	0.9248(5)	0.061(6)
O2	1	0.2949(7)	-0.0432(3)	0.8852(3)	0.020(3)
O3	1	-0.1438(7)	0.2290(4)	0.6744(4)	0.026(4)
O4	1	1.0627(8)	0.4041(4)	1.4034(4)	0.045(5)
O5	1	0.5994(7)	0.5180(4)	0.7836(4)	0.031(4)
O6	1	0.3229(7)	-0.1413(4)	1.0005(4)	0.032(4)
O7	1	0.8270(7)	0.1481(3)	1.1421(4)	0.022(3)
O8	1	0.6472(7)	0.4220(4)	0.7263(4)	0.030(4)
O9	1	0.1104(7)	0.3431(4)	0.7769(4)	0.035(4)
O10	1	0.8743(6)	-0.1702(3)	0.8138(3)	0.014(3)
O11	1	0.2926(9)	0.1003(5)	0.9638(5)	0.065(7)
O12	1	0.0066(8)	0.2304(4)	0.8216(4)	0.042(4)
O13	1	0.2516(8)	0.3441(4)	0.9116(4)	0.036(4)
O14	1	1.0729(6)	0.2700(3)	1.2526(3)	0.018(3)
O15	1	0.7139(7)	-0.0825(4)	0.7970(4)	0.031(4)
O16	1	0.5308(8)	0.0183(4)	0.7189(4)	0.041(4)
O17	1	0.5317(6)	0.1491(4)	0.8598(4)	0.026(4)
O18	1	0.7980(7)	0.4233(3)	0.8661(4)	0.030(3)
O19	1	0.6406(8)	0.3916(4)	0.9574(5)	0.049(6)
O20	1	0.7089(7)	0.5197(4)	0.7176(4)	0.037(4)
O21	1	1.0524(6)	0.5281(4)	1.2132(4)	0.033(4)
O22	1	0.407(1)	0.3521(5)	1.0613(6)	0.082(7)
O23	1	0.6567(8)	0.5427(3)	1.0382(3)	0.032(3)
O24	1	0.6394(8)	0.7243(5)	0.4641(5)	0.058(5)
O25	1	0.5170(7)	0.4579(4)	1.1014(4)	0.037(4)
O26	1	0.8177(6)	0.3317(4)	0.7414(3)	0.022(4)
O27	1	0.8214(8)	0.5840(3)	0.6920(4)	0.033(4)
O28	1	0.8221(8)	0.3501(5)	0.5012(5)	0.052(6)
O29	1	0.4674(8)	0.5197(4)	0.6399(4)	0.037(4)
O30	1	0.9638(7)	0.3321(3)	0.8813(4)	0.029(4)
O31	1	0.7903(8)	0.2733(4)	0.9576(4)	0.037(4)
O32	1	0.4988(6)	0.3973(4)	0.8172(4)	0.026(4)
O33	1	0.6543(9)	0.2770(5)	0.8169(5)	0.063(6)
O34	1	0.7196(7)	0.2269(3)	0.5376(3)	0.023(3)
O35	1	-0.1414(8)	0.1038(4)	0.5372(5)	0.049(5)
O36	1	0.5052(7)	0.2768(3)	0.6751(3)	0.026(4)
O37	1	0.8289(6)	0.0253(4)	1.0028(4)	0.022(4)
O38	1	0.2163(9)	0.2693(5)	0.3961(5)	0.059(5)
O39	1	0.2002(9)	0.4024(5)	0.5430(6)	0.072(8)
O40	1	0.6721(7)	0.0202(4)	0.8570(4)	0.033(4)
O41	1	0.8795(9)	0.0825(3)	0.7681(4)	0.042(4)
O42	1	0.9989(7)	0.1039(4)	0.6779(4)	0.028(4)
O43	1	0.0310(9)	0.0807(4)	0.9100(4)	0.047(5)
O44	1	0.0223(8)	-0.0265(4)	0.8576(4)	0.040(4)
O45	1	0.4255(7)	-0.0986(4)	0.7554(4)	0.035(5)
O46	1	0.746(1)	-0.1688(5)	0.6701(7)	0.121(9)
O47	1	0.5686(7)	-0.0982(3)	0.9006(4)	0.025(3)
O48	1	0.8073(7)	0.4707(3)	0.6434(3)	0.023(3)
O49	1	0.2297(8)	0.2934(4)	0.6515(4)	0.045(5)
O50	1	0.6711(8)	0.4552(4)	1.2367(4)	0.045(4)
O51	1	0.8780(7)	-0.0302(4)	0.7235(4)	0.033(4)
O52	1	0.323(1)	0.5262(5)	0.4947(5)	0.078(7)

O53	1	0.0308(9)	-0.1468(5)	0.7139(5)	0.059(6)
O54	1	0.784(1)	0.3973(6)	1.1111(7)	0.09(1)
O55	1	0.1393(9)	0.2293(5)	0.9642(5)	0.057(6)
O56	1	0.756(1)	0.2334(5)	0.7411(6)	0.081(8)
O57	1	0.2618(7)	0.2198(3)	1.1124(4)	0.029(4)
O58	1	0.2397(6)	0.1499(3)	0.5764(4)	0.019(3)
O59	1	0.3617(5)	0.3978(3)	0.6815(3)	0.006(3)
O60	1	0.7901(9)	0.5426(4)	1.1800(5)	0.057(6)
O61	1	0.7326(6)	-0.0283(3)	0.5783(3)	0.011(3)
O62	1	0.148(1)	0.0802(4)	1.0572(5)	0.064(6)
O63	1	0.2852(9)	0.3348(5)	1.1573(5)	0.059(6)
O64	1	0.932(1)	0.2716(4)	1.1057(5)	0.062(6)
O65	1	0.3762(6)	0.2947(3)	0.7951(3)	0.009(3)
O66	1	0.2837(6)	-0.1015(3)	0.6152(3)	0.012(3)
O67	1	-0.0375(7)	0.3495(4)	0.6394(4)	0.043(5)
O68	1	0.7234(9)	0.0820(4)	0.6255(5)	0.065(5)
O69	1	0.316(1)	-0.2088(5)	0.7182(5)	0.067(6)
O70	1	0.504(1)	0.1653(6)	0.6237(6)	0.098(9)
O71	1	0.4892(9)	0.4172(4)	0.5821(4)	0.049(5)
O72	1	0.6462(9)	0.1683(5)	0.7692(6)	0.080(7)
O73	1	1.0349(8)	0.4167(4)	1.1639(5)	0.063(5)
O74	1	0.1425(8)	0.0999(4)	0.8184(4)	0.040(4)
O75	1	0.3867(6)	0.1532(4)	0.7244(4)	0.032(4)
O76	1	0.9173(7)	0.4040(4)	1.2622(4)	0.034(4)
O77	1	0.146(1)	-0.0417(4)	0.7500(5)	0.077(6)
O78	1	-0.1629(8)	-0.0430(4)	0.4665(4)	0.045(4)
O79	1	0.1385(8)	0.2015(4)	0.6995(4)	0.040(4)
O80	1	0.568(1)	-0.0783(5)	0.6526(5)	0.069(6)
O81	1	-0.008(1)	-0.0366(5)	0.6063(5)	0.074(6)
O82	1	0.5493(7)	0.0467(4)	0.9778(4)	0.031(4)
O83	1	0.5204(8)	0.2902(4)	0.9379(4)	0.048(5)
O84	1	0.257(1)	0.2042(5)	0.8487(5)	0.069(6)
O85	1	0.5213(8)	0.2088(4)	1.1459(4)	0.041(4)
O86	1	0.857(1)	0.5232(6)	0.8648(5)	0.084(7)
O87	1	0.8024(9)	0.1668(4)	0.9086(4)	0.050(5)
O88	1	0.349(1)	0.4153(5)	0.4477(6)	0.084(7)
O89	1	-0.0198(8)	0.2057(4)	0.5615(4)	0.045(4)
O90	1	0.8960(7)	0.5198(4)	1.0697(4)	0.037(4)
O91	1	-0.031(1)	0.1684(5)	1.0436(5)	0.072(6)
O92	1	0.3974(9)	0.0163(4)	0.5691(5)	0.054(5)
O93	1	0.753(1)	0.6127(7)	1.2581(7)	0.10(1)
O94	1	0.572(2)	0.148(1)	1.066(1)	0.19
O95	1	1.0585(7)	0.5458(4)	1.4724(4)	0.033(4)
O96	1	0.708(1)	0.1390(6)	1.2037(5)	0.093(8)
O97	1	0.668(1)	0.3277(4)	0.5920(5)	0.062(6)
O98	1	0.125(1)	0.3345(4)	1.0218(5)	0.071(6)
O99	1	0.102(1)	0.2942(4)	0.5049(4)	0.067(5)
O1001		0.1698(9)	-0.2066(4)	0.5754(4)	0.044(4)
O1011		0.933(1)	0.0090(7)	0.9363(6)	0.109(9)
O1020.5		0.179(1)	0.2806(5)	1.1944(5)	0.006(5)
O1031		0.4062(9)	0.0433(4)	0.8313(4)	0.053(5)
O1041		0.578(2)	0.5163(9)	0.580(1)	0.19
O1050.5		0.2084(9)	0.6503(5)	0.7034(5)	0.000(4)
O1061		0.391(1)	0.3846(6)	0.8775(6)	0.095(8)
O1071		0.8345(8)	0.2914(3)	1.2116(4)	0.036(4)
O1081		0.934(1)	0.3662(8)	0.4445(7)	0.12(1)
O1091		0.1017(8)	0.1525(4)	0.4347(4)	0.042(5)
O1101		0.7824(6)	0.0241(4)	0.7988(3)	0.031(4)
O1111		0.282(1)	0.0445(5)	0.6823(6)	0.114(9)
O1121		0.927(1)	0.5466(5)	1.3243(5)	0.084(7)
O1131		0.5442(7)	0.3549(4)	1.2162(4)	0.036(5)
O1141		0.963(1)	0.2950(4)	1.3612(5)	0.068(6)
O1151		0.671(1)	0.2863(5)	1.0759(5)	0.078(6)
O1161		0.8967(8)	0.2373(5)	0.8824(5)	0.060(6)
O1171		0.605(1)	0.2303(5)	0.6040(6)	0.084(8)
O1180.5		0.179(8)	0.606(4)	0.672(3)	0.53(9)

O1191		0.038(1)	-0.1073(6)	0.5301(5)	0.089(8)
O1201		0.1010(6)	0.1016(3)	0.6102(4)	0.021(3)
O1210.5		0.3517(8)	0.2060(4)	1.0060(3)	-0.018(3)
O1221		0.627(2)	0.011(1)	0.651(1)	0.19
O1231		0.5450(8)	0.3938(4)	1.0240(4)	0.040(4)
O1240.5		0.0399(9)	0.2740(5)	1.0481(6)	0.000(5)
O1250.5		0.2283(8)	0.1002(5)	0.7517(4)	0.002(4)
O1260.5		0.158(1)	-0.1394(6)	0.6634(7)	0.023(7)
O1271		0.416(1)	-0.0879(6)	0.5119(6)	0.096(8)
O1281		0.612(1)	0.8314(5)	0.5195(5)	0.067(6)
O1290.5		0.878(1)	0.4168(6)	1.0236(6)	0.007(5)
O1300.5		0.944(1)	0.4201(5)	1.0105(6)	0.007(5)
O1311		0.417(2)	0.136(1)	0.919(1)	0.195(1)
O1321		0.668(2)	0.374(1)	1.161(1)	0.19
O1330.5		0.177(1)	-0.1050(7)	0.6693(8)	0.027(7)
O1340.5		0.064(1)	0.3534(5)	0.5849(7)	0.021(6)
O1350.5		0.1036(7)	0.3942(4)	0.6014(4)	-0.015(3)
O1360.5		0.4265(6)	0.2054(3)	0.9883(4)	-0.013(3)
O1370.5		1.0100(7)	0.4777(4)	0.9950(4)	-0.017(3)
O1380.5		0.043(2)	0.2361(6)	1.0240(8)	0.033(8)
O1391		0.188(1)	0.5434(4)	0.6178(5)	0.055(5)
O1400.5		0.671(2)	0.7260(6)	0.666(1)	0.07(1)
O1411		0.574(1)	0.6654(4)	0.6984(5)	0.065(6)
O1421		0.5899(8)	0.7808(4)	0.7489(4)	0.041(5)
O1431		0.4395(9)	0.7770(4)	0.6028(5)	0.051(5)
O1441		0.455(1)	0.6721(6)	0.5528(7)	0.11(1)
O1451		0.553(1)	0.7392(9)	0.5284(8)	0.14(1)
O1460.5		0.520(2)	0.984(1)	0.496(1)	0.08(2)
O1480.5		0.156(2)	0.241(1)	0.175(1)	0.095(1)
O1490.5		0.680(4)	0.780(2)	0.690(2)	0.19
O1500.5		0.2858(9)	0.141(1)	0.7789(9)	0.09(1)
B1	1	0.3150(9)	0.6405(4)	0.6356(5)	0.045(5)
B2	1	0.3473(8)	-0.1531(4)	0.7545(5)	0.000(4)
B3	1	-0.036(1)	-0.1040(9)	0.5650(7)	0.040(8)
B4	1	0.1327(5)	0.0196(3)	1.0439(3)	-0.025(2)
B5	1	0.136(1)	0.3571(5)	0.5478(4)	0.009(4)
B6	1	0.786(1)	0.5237(6)	0.6791(8)	0.042(7)
B7	1	0.2767(9)	0.3555(6)	0.6838(5)	0.008(5)
B8	1	0.6498(7)	0.4875(4)	0.7427(3)	-0.008(3)
B9	1	0.8492(8)	0.3549(4)	1.2557(4)	-0.003(3)
B10	1	0.4408(8)	0.3602(4)	0.8279(5)	0.008(4)
B11	1	0.841(1)	0.0223(5)	0.7561(7)	0.028(6)
B12	1	0.0852(7)	0.1405(5)	0.6727(5)	0.004(4)
B13	1	0.7306(6)	-0.0173(3)	0.8232(4)	-0.013(3)
B14	1	0.193(2)	-0.143(1)	0.6152(8)	0.07(1)
B15	1	0.8192(8)	0.2180(5)	0.9099(4)	0.000(4)
B16	1	0.8010(9)	0.4796(5)	0.8850(5)	0.006(4)
B17	1	-0.057(1)	0.1432(7)	0.5283(7)	0.037(7)
B18	1	0.4763(9)	0.3955(5)	1.0571(5)	0.006(4)
B19	1	0.879(1)	-0.2312(8)	0.7798(8)	0.039(8)
B20	1	-0.014(1)	0.0200(5)	0.8948(4)	0.010(4)
B21	1	0.5025(7)	0.1464(3)	1.1005(4)	-0.011(3)
B22	1	0.751(1)	-0.2333(7)	0.6477(7)	0.031(7)
B23	1	0.6818(8)	0.2685(4)	0.5791(4)	-0.001(3)
B24	1	-0.011(1)	0.2330(4)	1.0631(4)	0.011(4)
B25	1	0.308(1)	0.0999(6)	0.7165(6)	0.018(5)
B26	1	0.122(1)	-0.1002(8)	0.7195(6)	0.030(7)
B27	1	0.2461(6)	0.2708(3)	1.1458(3)	-0.018(2)
B28	1	0.8944(9)	0.3984(8)	0.4971(7)	0.031(7)
B29	1	0.6176(7)	0.3969(5)	1.2069(4)	-0.003(4)
B30	1	0.816(1)	0.6068(6)	1.2167(5)	0.007(5)
B31	1	0.5203(8)	0.4780(5)	0.6022(5)	-0.001(4)
B32	1	0.5337(9)	0.2256(6)	0.6365(5)	0.012(5)
B33	1	0.367(1)	0.1473(8)	0.9646(8)	0.037(8)
B34	1	0.051(1)	0.3936(7)	0.6428(7)	0.027(6)
B35	1	0.5579(6)	0.3519(3)	0.9684(3)	-0.016(2)

B36	1	1.0871(7)	0.4796(4)	1.1727(4)	-0.007(3)
B37	1	0.6995(7)	0.0219(4)	0.6175(3)	-0.010(3)
B38	1	0.982(1)	0.3593(7)	1.4058(6)	0.026(6)
B39	1	0.944(1)	0.4825(5)	1.0327(5)	0.019(5)
B40	1	0.4576(8)	0.1035(4)	0.8671(5)	0.002(4)
B41	1	0.434(1)	-0.0257(5)	0.5259(5)	0.013(5)
B42	1	0.962(1)	0.2692(5)	0.8617(4)	0.018(4)
B43	1	0.7453(8)	0.1064(4)	1.1513(4)	-0.007(3)
B44	1	0.7146(9)	0.3506(5)	1.1050(5)	0.006(4)
B45	1	0.6655(8)	0.5986(5)	1.0725(6)	0.015(5)
B46	1	0.225(1)	0.1449(5)	0.8161(6)	0.023(5)
B47	1	0.366(1)	0.4799(7)	0.4635(6)	0.021(6)
B48	1	0.113(1)	0.2747(7)	1.0122(6)	0.028(6)
B49	1	0.678(1)	0.2345(8)	0.7780(7)	0.040(7)
B50	1	0.626(2)	0.734(1)	0.704(2)	0.19(3)
B51	1	0.477(2)	0.7295(9)	0.5550(6)	0.044(8)
B52	1	0.850(4)	0.906(2)	0.434(2)	0.19
B53	1	0.592(4)	0.100(2)	1.007(2)	0.19
B54	1	0.603(3)	0.774(1)	0.505(1)	0.09(1)
B55	1	0.233(2)	0.6131(9)	0.651(1)	0.038(8)
B56	1	0.197(3)	0.733(1)	0.288(2)	0.13(2)
B57	1	0.569(2)	-0.021(1)	0.666(1)	0.09(1)

Table S34 Anisotropic parameters of atomic displacements (Å^2) in in the supercell structure of $Ca_2B_2O_5$ at 810 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.031(2)	0.035(2)	0.017(1)	0.008(1)	0.003(1)	0.016(1)
Ca2	0.012(1)	0.011(1)	0.019(1)	-0.0024(8)	0.0044(9)	0.0028(9)
Ca3	0.038(2)	0.011(1)	0.022(1)	0.008(1)	0.003(1)	-0.002(1)
Ca4	0.024(1)	0.034(2)	0.029(2)	0.008(1)	0.004(1)	0.026(1)
Ca5	0.045(2)	0.019(1)	0.017(1)	0.008(1)	0.003(1)	0.010(1)
Ca6	0.041(2)	0.033(2)	0.026(2)	0.016(1)	0.003(1)	0.023(1)
Ca7	0.032(1)	0.016(1)	0.013(1)	-0.016(1)	-0.007(1)	0.003(1)
Ca8	0.026(1)	0.028(1)	0.015(1)	-0.013(1)	-0.004(1)	0.014(1)
Ca9	0.020(1)	0.018(1)	0.006(1)	0.010(1)	-0.0074(9)	-0.0002(9)
Ca10	0.034(1)	0.021(1)	0.019(1)	0.018(1)	0.007(1)	0.008(1)
Ca11	0.041(2)	0.013(1)	0.015(1)	-0.008(1)	-0.008(1)	0.008(1)
Ca12	0.024(1)	0.014(1)	0.012(1)	0.004(1)	0.002(1)	0.001(1)
Ca13	0.017(1)	0.025(1)	0.033(2)	-0.000(1)	-0.008(1)	0.011(1)
Ca14	0.035(2)	0.054(2)	0.017(1)	0.021(1)	0.006(1)	0.026(1)
Ca15	0.037(2)	0.017(1)	0.011(1)	0.013(1)	0.012(1)	-0.008(1)
Ca16	0.029(1)	0.023(1)	0.029(1)	0.002(1)	0.015(1)	0.022(1)
Ca17	0.029(2)	0.026(1)	0.025(2)	-0.008(1)	-0.031(1)	0.015(1)
Ca18	0.033(1)	0.025(1)	0.013(1)	-0.007(1)	-0.000(1)	0.013(1)
Ca19	0.044(2)	0.027(2)	0.034(2)	0.022(1)	0.013(1)	0.017(1)
Ca20	0.044(2)	0.019(1)	0.014(1)	0.010(1)	0.013(1)	-0.000(1)
Ca21	0.040(2)	0.015(1)	0.023(1)	-0.001(1)	0.007(1)	0.010(1)
Ca22	0.030(1)	0.006(1)	0.033(2)	-0.0121(9)	-0.014(1)	0.016(1)
Ca23	0.032(2)	0.022(1)	0.043(2)	0.007(1)	-0.002(1)	0.021(1)
Ca24	0.026(1)	0.011(1)	0.011(1)	0.0066(9)	0.007(1)	0.0001(9)
Ca25	0.023(1)	0.004(1)	0.039(2)	-0.0059(9)	-0.009(1)	0.008(1)
Ca26	0.022(1)	0.011(1)	0.011(1)	-0.0106(9)	0.0013(9)	0.0016(9)
Ca27	0.039(2)	0.025(1)	0.017(1)	0.020(1)	-0.001(1)	0.005(1)
Ca28	0.054(2)	0.011(1)	0.014(1)	0.015(1)	0.000(1)	-0.004(1)
Ca29	0.037(2)	0.021(1)	0.013(1)	-0.006(1)	0.002(1)	0.004(1)
Ca30	0.021(1)	0.026(1)	0.012(1)	0.011(1)	0.002(1)	-0.001(1)
Ca31	0.036(2)	0.027(1)	0.021(1)	0.003(1)	-0.001(1)	0.018(1)
Ca32	0.050(2)	0.034(2)	0.025(2)	0.003(1)	0.008(1)	0.016(1)
Ca33	0.046(2)	0.016(1)	0.005(1)	0.005(1)	-0.000(1)	0.002(1)
Ca34	0.069(2)	0.026(2)	0.023(2)	0.021(1)	0.007(2)	0.014(1)
Ca35	0.051(2)	0.033(2)	0.031(2)	0.024(1)	0.009(1)	0.020(1)
Ca36	0.034(2)	0.021(1)	0.017(1)	0.012(1)	0.007(1)	0.005(1)
Ca37	0.029(1)	0.022(1)	0.015(1)	-0.004(1)	-0.002(1)	0.007(1)
Ca38	0.055(2)	0.007(1)	0.009(1)	-0.009(1)	-0.004(1)	-0.006(1)
Ca39	0.030(3)	0.027(1)	0.023(1)	0.013(1)	-0.021(1)	0.003(1)

Ca40	0.025(1)	0.036(2)	0.039(2)	0.002(1)	-0.022(1)	0.034(1)
Ca41	0.033(3)	0.014(1)	0.023(1)	-0.008(1)	-0.013(1)	0.011(1)
Ca42	0.046(2)	0.008(1)	0.006(1)	0.021(1)	0.002(1)	-0.0018(9)
Ca43	0.039(2)	0.026(1)	0.037(2)	0.019(1)	0.023(1)	0.026(1)
Ca44	0.011(1)	0.025(1)	0.013(1)	-0.0111(9)	-0.0106(9)	0.010(1)
Ca45	0.058(2)	0.022(1)	0.009(1)	0.014(1)	0.005(1)	0.003(1)
Ca46	0.027(2)	0.040(2)	0.056(2)	-0.011(1)	-0.009(1)	0.035(2)
Ca47	0.060(2)	0.029(2)	0.019(2)	0.029(2)	-0.003(1)	0.004(1)
Ca48	0.056(2)	0.015(1)	0.017(1)	-0.000(1)	-0.002(1)	-0.003(1)
Ca49	0.038(2)	0.012(1)	0.010(1)	-0.015(1)	-0.017(1)	0.000(1)
Ca50	0.017(1)	0.025(1)	0.037(2)	-0.001(1)	-0.007(1)	0.030(1)
Ca51	0.063(2)	0.026(2)	0.007(1)	0.012(1)	-0.028(1)	-0.003(1)
Ca52	0.024(1)	0.031(2)	0.038(2)	0.001(1)	0.005(1)	0.026(1)
Ca53	0.018(1)	0.016(1)	0.022(1)	0.004(1)	-0.006(1)	0.004(1)
Ca54	0.055(2)	0.026(2)	0.029(2)	-0.010(1)	-0.025(1)	0.013(1)
Ca55	0.032(2)	0.025(1)	0.036(2)	-0.003(1)	0.011(1)	0.014(1)
Ca56	0.097(3)	0.039(2)	0.025(2)	0.047(2)	0.023(2)	0.016(1)
O1	0.11(1)	0.020(5)	0.041(7)	0.023(6)	0.036(7)	-0.002(5)
O2	0.045(5)	0.004(3)	0.020(4)	0.005(3)	0.002(4)	0.016(3)
O3	0.028(5)	0.017(4)	0.021(5)	0.012(4)	0.005(4)	-0.003(4)
O4	0.042(6)	0.030(5)	0.050(7)	-0.002(4)	0.005(5)	0.014(5)
O5	0.035(5)	0.036(5)	0.023(5)	0.008(4)	0.026(4)	0.005(4)
O6	0.039(5)	0.021(4)	0.025(5)	-0.014(4)	0.009(4)	0.006(4)
O7	0.027(4)	0.018(4)	0.028(5)	0.000(3)	0.026(4)	0.009(4)
O8	0.026(5)	0.024(5)	0.028(5)	0.005(4)	-0.007(4)	0.008(4)
O9	0.033(5)	0.054(6)	0.027(5)	-0.002(4)	0.014(4)	0.026(5)
O10	0.019(4)	0.017(4)	0.020(4)	0.014(3)	0.006(3)	0.019(3)
O11	0.043(6)	0.067(8)	0.09(1)	-0.002(6)	0.036(7)	0.043(7)
O12	0.056(6)	0.031(5)	0.003(4)	0.002(5)	-0.005(4)	-0.018(4)
O13	0.054(6)	0.018(4)	0.040(6)	0.009(4)	0.024(5)	0.012(4)
O14	0.004(3)	0.028(4)	0.016(4)	0.011(3)	0.005(3)	0.002(4)
O15	0.042(5)	0.019(4)	0.032(5)	0.016(4)	0.017(4)	0.006(4)
O16	0.053(6)	0.024(5)	0.037(6)	-0.005(4)	0.028(5)	0.001(4)
O17	0.017(4)	0.026(4)	0.044(6)	-0.009(3)	0.006(4)	0.030(4)
O18	0.035(5)	0.002(4)	0.021(5)	-0.013(3)	-0.001(4)	-0.016(3)
O19	0.033(5)	0.057(6)	0.088(9)	0.014(5)	0.035(6)	0.053(6)
O20	0.035(5)	0.045(6)	0.044(6)	-0.003(4)	0.015(5)	0.033(5)
O21	0.004(4)	0.045(5)	0.035(5)	-0.020(3)	-0.012(4)	0.017(5)
O22	0.093(9)	0.064(8)	0.09(1)	-0.026(7)	0.018(8)	0.052(8)
O23	0.061(6)	0.003(4)	0.000(4)	0.001(4)	-0.018(4)	-0.015(3)
O24	0.031(6)	0.062(7)	0.036(6)	-0.022(5)	0.013(5)	-0.013(5)
O25	0.041(6)	0.022(5)	0.029(5)	-0.005(4)	-0.015(4)	0.009(4)
O26	0.025(4)	0.035(5)	0.018(4)	0.024(4)	0.013(4)	0.016(4)
O27	0.064(6)	0.005(4)	0.023(5)	0.009(4)	0.001(4)	0.007(4)
O28	0.041(6)	0.082(8)	0.071(8)	0.023(6)	0.022(6)	0.064(7)
O29	0.036(5)	0.045(6)	0.035(6)	0.005(4)	0.020(5)	0.020(5)
O30	0.041(5)	0.008(4)	0.026(5)	0.004(4)	-0.007(4)	0.005(4)
O31	0.044(6)	0.042(5)	0.023(5)	0.035(5)	0.020(4)	0.002(4)
O32	0.009(4)	0.035(5)	0.050(6)	0.007(3)	0.023(4)	0.028(5)
O33	0.049(7)	0.073(8)	0.049(8)	0.013(6)	-0.009(6)	0.021(7)
O34	0.035(5)	0.021(4)	0.011(4)	0.012(4)	0.003(4)	0.005(4)
O35	0.048(6)	0.039(6)	0.076(8)	-0.002(5)	0.029(6)	0.037(6)
O36	0.050(5)	0.021(4)	0.016(4)	0.040(4)	0.025(4)	0.000(3)
O37	0.013(4)	0.037(5)	0.026(5)	0.014(4)	0.011(4)	0.019(4)
O38	0.064(7)	0.047(7)	0.044(7)	-0.006(6)	0.025(6)	0.003(6)
O39	0.060(7)	0.084(9)	0.14(1)	0.041(7)	0.065(8)	0.085(9)
O40	0.041(5)	0.025(5)	0.041(6)	0.040(4)	0.020(5)	0.010(4)
O41	0.095(8)	0.000(4)	0.013(4)	0.002(4)	-0.009(5)	-0.002(3)
O42	0.038(5)	0.035(5)	0.027(5)	0.005(4)	0.020(4)	0.026(4)
O43	0.069(7)	0.028(5)	0.026(5)	0.000(5)	-0.011(5)	0.010(4)
O44	0.053(6)	0.033(5)	0.012(4)	-0.012(4)	0.004(4)	-0.003(4)
O45	0.019(4)	0.058(6)	0.058(7)	0.020(4)	0.020(5)	0.048(6)
O46	0.17(2)	0.012(6)	0.14(1)	0.034(8)	0.01(1)	0.004(7)
O47	0.034(5)	0.006(4)	0.029(5)	-0.002(3)	0.001(4)	0.009(4)
O48	0.055(6)	0.011(4)	0.007(4)	0.013(4)	0.020(4)	0.001(3)
O49	0.049(6)	0.029(5)	0.042(6)	-0.006(5)	0.006(5)	0.009(5)

O50	0.044(6)	0.025(5)	0.037(6)	-0.014(4)	-0.026(5)	0.013(5)
O51	0.024(5)	0.038(5)	0.043(6)	0.020(4)	0.011(4)	0.019(5)
O52	0.10(1)	0.054(7)	0.061(8)	0.049(7)	0.026(8)	0.001(6)
O53	0.048(7)	0.058(7)	0.072(9)	0.019(6)	0.019(6)	0.028(7)
O54	0.08(1)	0.11(1)	0.15(1)	-0.001(8)	0.05(1)	0.09(1)
O55	0.059(7)	0.047(6)	0.058(7)	0.022(6)	0.036(6)	0.006(6)
O56	0.075(9)	0.062(8)	0.12(1)	0.048(7)	0.033(9)	0.039(8)
O57	0.036(5)	0.011(4)	0.024(5)	0.002(4)	-0.002(4)	-0.003(4)
O58	0.007(3)	0.011(4)	0.044(5)	-0.008(3)	0.011(4)	0.017(4)
O59	0.000(3)	-0.002(3)	0.024(4)	-0.001(2)	0.007(3)	0.007(3)
O60	0.073(8)	0.028(6)	0.060(8)	0.004(5)	0.021(6)	0.012(5)
O61	0.022(4)	0.003(3)	-0.004(3)	0.002(3)	0.003(3)	-0.012(3)
O62	0.086(8)	0.024(5)	0.058(7)	0.007(5)	-0.028(6)	0.020(5)
O63	0.071(8)	0.061(7)	0.044(7)	0.005(6)	0.001(6)	0.032(6)
O64	0.081(9)	0.034(6)	0.056(8)	0.015(6)	0.019(7)	0.006(6)
O65	0.021(4)	-0.005(3)	0.002(3)	-0.005(3)	0.004(3)	-0.007(3)
O66	0.003(3)	0.007(3)	0.016(4)	-0.012(3)	-0.008(3)	0.005(3)
O67	0.021(5)	0.049(6)	0.068(7)	-0.024(4)	-0.008(5)	0.052(6)
O68	0.082(8)	0.002(4)	0.056(7)	-0.002(5)	-0.043(6)	-0.002(4)
O69	0.10(1)	0.048(7)	0.033(6)	0.011(6)	-0.022(6)	0.024(6)
O70	0.12(1)	0.068(9)	0.12(1)	0.008(8)	0.01(1)	0.070(9)
O71	0.078(8)	0.014(5)	0.039(6)	0.007(5)	-0.007(6)	0.009(4)
O72	0.060(8)	0.056(7)	0.09(1)	-0.032(6)	-0.029(7)	0.047(7)
O73	0.063(7)	0.006(4)	0.068(8)	-0.032(4)	-0.035(6)	0.004(5)
O74	0.040(6)	0.029(5)	0.035(6)	0.004(4)	-0.004(5)	0.008(5)
O75	0.000(4)	0.038(5)	0.063(7)	-0.005(3)	0.009(4)	0.028(5)
O76	0.036(5)	0.046(6)	0.029(5)	0.003(4)	0.000(4)	0.032(5)
O77	0.11(1)	0.009(5)	0.067(9)	-0.006(6)	0.004(8)	-0.004(5)
O78	0.056(6)	0.010(4)	0.038(6)	-0.016(4)	-0.015(5)	0.000(4)
O79	0.051(6)	0.028(5)	0.039(6)	0.014(5)	0.011(5)	0.014(5)
O80	0.086(9)	0.034(6)	0.043(7)	0.000(6)	-0.016(6)	-0.002(5)
O81	0.09(1)	0.042(7)	0.045(7)	-0.012(6)	-0.024(7)	0.010(6)
O82	0.020(4)	0.035(5)	0.014(4)	-0.016(4)	-0.021(4)	0.009(4)
O83	0.054(6)	0.025(5)	0.051(7)	-0.001(5)	-0.015(5)	0.022(5)
O84	0.088(9)	0.033(6)	0.058(8)	-0.013(6)	-0.015(7)	0.019(6)
O85	0.047(6)	0.020(5)	0.038(6)	0.011(4)	0.000(5)	0.003(4)
O86	0.078(8)	0.12(1)	0.055(8)	0.010(8)	0.062(7)	0.019(7)
O87	0.064(7)	0.043(6)	0.038(6)	-0.004(5)	-0.012(5)	0.031(5)
O88	0.13(1)	0.022(6)	0.09(1)	0.029(7)	0.033(9)	0.025(7)
O89	0.049(6)	0.030(5)	0.028(5)	-0.006(4)	-0.034(5)	0.012(5)
O90	0.035(5)	0.056(6)	0.019(5)	0.020(5)	0.006(4)	0.013(5)
O91	0.13(1)	0.038(6)	0.051(7)	0.042(7)	0.016(8)	0.025(6)
O92	0.062(7)	0.041(6)	0.039(6)	0.020(5)	0.011(6)	-0.003(5)
O93	0.065(9)	0.15(1)	0.12(1)	0.026(9)	0.050(9)	0.08(1)
O94	0.19	0.19	0.19	0.044633	0.055162	0.085769
O95	0.034(5)	0.025(5)	0.030(5)	0.004(4)	-0.019(4)	0.018(4)
O96	0.09(1)	0.12(1)	0.050(8)	0.007(8)	0.058(8)	0.018(8)
O97	0.081(8)	0.029(6)	0.068(8)	0.024(6)	-0.004(7)	0.025(6)
O98	0.12(1)	0.001(4)	0.074(8)	-0.003(5)	0.003(8)	0.019(5)
O99	0.099(9)	0.016(5)	0.037(6)	-0.012(5)	-0.041(6)	0.000(5)
O100	0.077(7)	0.010(4)	0.029(6)	0.010(5)	0.003(5)	0.001(4)
O101	0.09(1)	0.15(1)	0.08(1)	-0.006(9)	0.070(9)	0.04(1)
O102	0.033(8)	-0.006(5)	0.006(6)	-0.003(5)	0.040(6)	-0.002(5)
O103	0.099(9)	0.002(4)	0.028(5)	-0.008(5)	-0.020(5)	0.003(4)
O104	0.19	0.19	0.19	0.044633	0.055162	0.085769
O105	-0.009(5)	0.001(5)	-0.008(5)	-0.021(4)	-0.007(4)	-0.009(4)
O106	0.10(1)	0.12(1)	0.07(1)	0.036(9)	0.069(9)	0.023(9)
O107	0.065(6)	0.006(4)	0.014(4)	0.006(4)	0.009(4)	-0.014(3)
O108	0.13(1)	0.19(2)	0.11(1)	0.09(1)	0.09(1)	0.09(1)
O109	0.059(7)	0.024(5)	0.047(6)	0.003(5)	0.022(5)	0.018(5)
O110	0.024(4)	0.071(6)	0.021(4)	0.013(4)	0.026(4)	0.034(5)
O111	0.16(1)	0.041(8)	0.09(1)	0.014(8)	-0.05(1)	0.024(8)
O112	0.10(1)	0.051(7)	0.060(9)	-0.008(7)	-0.041(7)	0.024(7)
O113	0.011(4)	0.054(6)	0.058(7)	0.007(4)	0.021(4)	0.035(5)
O114	0.095(9)	0.028(6)	0.054(8)	0.005(6)	-0.020(7)	0.016(6)
O115	0.11(1)	0.041(6)	0.037(7)	0.025(7)	-0.048(7)	0.003(5)

O116	0.053(7)	0.070(7)	0.090(9)	0.010(6)	0.057(7)	0.050(7)
O117	0.11(1)	0.043(7)	0.11(1)	0.009(7)	0.08(1)	0.027(7)
O118	0.6(2)	0.5(1)	0.25(8)	0.27(11)	-0.28(9)	0.05(8)
O119	0.11(1)	0.11(1)	0.074(9)	0.040(9)	0.083(9)	0.044(8)
O120	0.012(4)	0.006(3)	0.043(5)	-0.010(3)	0.023(4)	0.004(3)
O121	0.005(5)	-0.019(4)	-0.028(3)	0.016(4)	0.012(3)	-0.011(3)
O122	0.19	0.19	0.19	0.044633	0.055162	0.085769
O123	0.038(5)	0.033(5)	0.045(6)	0.011(4)	0.026(5)	0.006(4)
O124	0.001(5)	-0.022(5)	0.028(8)	0.006(4)	0.009(5)	0.003(5)
O125	-0.015(5)	0.001(5)	-0.016(4)	-0.044(4)	-0.013(4)	-0.021(4)
O126	0.027(8)	-0.006(6)	0.07(1)	0.001(6)	0.069(9)	0.007(7)
O127	0.13(1)	0.061(8)	0.07(1)	0.016(8)	0.009(9)	0.022(8)
O128	0.10(1)	0.032(6)	0.041(7)	0.017(6)	-0.005(7)	0.004(5)
O129	-0.013(5)	0.024(8)	0.010(7)	-0.015(5)	-0.010(5)	0.018(6)
O130	0.005(6)	-0.024(4)	0.011(7)	-0.010(4)	-0.028(5)	-0.014(4)
O131	0.18(2)	0.27(2)	0.26(3)	0.17(2)	0.14(2)	0.17(2)
O132	0.19	0.19	0.19	0.044633	0.055162	0.085769
O133	0.012(8)	0.002(7)	0.04(1)	-0.029(6)	-0.029(7)	0.015(7)
O134	0.018(7)	-0.016(5)	0.04(1)	-0.009(5)	0.015(7)	-0.010(6)
O135	-0.016(4)	-0.013(4)	-0.020(4)	-0.013(3)	0.012(3)	-0.018(3)
O136	-0.029(3)	-0.032(3)	-0.011(4)	-0.037(3)	-0.021(3)	-0.025(3)
O137	-0.009(4)	-0.023(3)	-0.014(4)	0.005(3)	-0.006(3)	-0.006(3)
O138	0.08(1)	-0.009(7)	0.06(1)	0.005(7)	0.04(1)	0.021(8)
O139	0.093(9)	0.020(5)	0.050(7)	-0.005(5)	0.009(6)	0.026(5)
O140	0.15(2)	-0.031(5)	0.08(2)	-0.006(8)	0.06(2)	-0.004(7)
O141	0.077(8)	0.024(6)	0.088(9)	0.004(5)	0.002(7)	0.031(6)
O142	0.060(7)	0.042(6)	0.032(5)	0.037(5)	0.043(5)	0.006(5)
O143	0.059(7)	0.026(5)	0.055(7)	0.004(5)	0.037(6)	-0.003(5)
O144	0.18(2)	0.052(9)	0.09(1)	0.036(9)	0.02(1)	0.037(9)
O145	0.08(1)	0.21(2)	0.13(2)	0.05(1)	0.04(1)	0.09(2)
O146	0.08(2)	0.06(2)	0.09(2)	0.04(1)	0.05(2)	0.04(2)
O148	0.11(2)	0.07(2)	0.04(2)	0.03(2)	-0.01(2)	-0.02(1)
O149	0.19	0.19	0.19	0.044633	0.055162	0.085769
O150	-0.037(5)	0.23(3)	0.05(1)	-0.036(9)	0.006(6)	0.06(2)
B1	0.069(7)	0.010(4)	0.060(7)	0.000(4)	0.013(6)	0.025(5)
B2	0.003(5)	-0.016(4)	0.009(5)	0.002(3)	-0.013(4)	0.000(4)
B3	0.012(7)	0.08(1)	0.032(9)	-0.005(7)	0.007(7)	0.029(9)
B4	-0.033(2)	-0.023(3)	-0.020(3)	-0.004(2)	-0.010(2)	-0.009(2)
B5	0.018(6)	0.023(6)	-0.021(4)	-0.001(5)	-0.017(4)	0.003(4)
B6	0.05(1)	-0.007(5)	0.05(1)	-0.015(6)	-0.036(8)	0.008(6)
B7	-0.003(5)	0.025(6)	0.018(6)	0.005(4)	0.006(4)	0.021(6)
B8	-0.002(4)	-0.009(4)	-0.023(3)	-0.006(3)	-0.007(3)	-0.015(3)
B9	0.006(5)	-0.006(4)	-0.016(3)	0.007(4)	-0.007(3)	-0.010(3)
B10	-0.002(4)	-0.016(4)	0.023(6)	-0.017(3)	-0.025(4)	0.000(4)
B11	0.033(8)	-0.004(5)	0.044(9)	0.005(5)	-0.003(7)	0.004(6)
B12	-0.019(4)	0.015(5)	0.002(5)	-0.007(4)	-0.010(3)	-0.005(4)
B13	-0.024(3)	-0.012(3)	-0.002(4)	-0.002(2)	-0.003(3)	-0.002(3)
B14	0.09(2)	0.06(1)	0.018(9)	0.04(1)	-0.02(1)	-0.017(9)
B15	-0.010(4)	0.010(5)	-0.001(4)	-0.007(3)	-0.007(3)	0.006(4)
B16	0.002(5)	0.008(5)	0.012(6)	-0.005(4)	-0.003(4)	0.014(5)
B17	0.027(8)	0.022(8)	0.04(1)	0.013(6)	0.022(7)	-0.013(7)
B18	0.012(5)	0.002(5)	0.002(5)	-0.004(4)	-0.013(4)	0.008(4)
B19	-0.007(5)	0.05(1)	0.06(1)	0.011(6)	-0.027(6)	0.023(9)
B20	0.029(7)	0.005(5)	-0.011(4)	-0.002(5)	-0.004(4)	-0.004(4)
B21	-0.005(4)	-0.021(3)	0.002(4)	-0.007(3)	0.007(3)	0.001(3)
B22	0.05(1)	0.025(8)	0.017(7)	0.010(7)	-0.006(7)	0.018(7)
B23	0.000(4)	-0.005(4)	0.002(5)	-0.001(3)	0.006(4)	-0.002(4)
B24	0.030(7)	-0.014(4)	-0.010(4)	-0.003(4)	-0.017(4)	-0.021(3)
B25	0.013(6)	0.008(6)	0.024(7)	0.007(5)	0.006(5)	-0.002(5)
B26	0.014(6)	0.08(1)	0.013(7)	0.032(7)	0.017(6)	0.029(8)
B27	-0.023(3)	-0.024(3)	-0.010(3)	-0.008(2)	-0.015(2)	-0.005(3)
B28	-0.010(5)	0.07(1)	0.05(1)	0.012(6)	-0.018(5)	0.054(9)
B29	-0.009(4)	0.018(5)	0.009(5)	0.007(4)	0.007(4)	0.027(5)
B30	0.016(6)	0.029(7)	-0.002(5)	0.020(5)	0.015(4)	0.016(5)
B31	-0.012(4)	0.003(5)	0.005(5)	-0.004(3)	-0.009(3)	0.006(4)
B32	0.000(5)	0.029(7)	0.023(6)	-0.011(4)	0.007(5)	0.029(6)

B33	0.012(7)	0.06(1)	0.06(1)	0.009(7)	0.014(8)	0.04(1)
B34	0.024(7)	0.037(9)	0.026(8)	0.016(7)	0.018(7)	0.011(7)
B35	-0.018(3)	-0.027(3)	-0.011(3)	-0.003(2)	-0.006(3)	-0.016(2)
B36	-0.016(3)	-0.002(4)	-0.013(3)	0.008(3)	0.002(3)	-0.018(3)
B37	-0.008(4)	-0.005(4)	-0.018(3)	-0.011(3)	0.009(3)	-0.011(3)
B38	0.025(7)	0.042(8)	0.004(6)	0.024(7)	-0.024(5)	0.013(6)
B39	0.046(9)	0.008(6)	0.009(6)	0.006(6)	0.029(6)	0.001(5)
B40	0.000(4)	-0.005(4)	0.036(7)	0.004(4)	0.012(5)	0.025(5)
B41	0.038(7)	0.011(6)	0.013(6)	0.014(5)	0.039(6)	0.010(5)
B42	0.043(8)	0.002(5)	-0.015(4)	0.001(5)	-0.034(5)	-0.006(4)
B43	-0.001(4)	0.001(4)	-0.018(3)	-0.005(3)	-0.004(3)	0.000(3)
B44	0.010(5)	0.018(6)	-0.001(5)	0.007(4)	0.014(4)	0.005(4)
B45	-0.014(4)	-0.002(5)	0.043(8)	-0.010(3)	0.003(5)	-0.005(5)
B46	0.051(9)	0.000(5)	0.004(6)	-0.003(6)	0.004(6)	-0.009(5)
B47	0.008(6)	0.047(8)	0.018(7)	0.025(6)	0.023(5)	0.009(6)
B48	0.030(8)	0.041(9)	0.013(7)	-0.002(7)	0.013(6)	0.009(6)
B49	0.028(9)	0.04(1)	0.009(7)	-0.022(7)	-0.026(6)	-0.003(7)
B50	0.00(1)	0.13(3)	0.31(5)	-0.06(1)	-0.13(2)	0.09(3)
B51	0.033(9)	0.07(1)	0.006(7)	0.033(9)	-0.003(6)	-0.008(7)
B52	0.19	0.19	0.19	0.044633	0.055162	0.085769
B53	0.19	0.19	0.19	0.044633	0.055162	0.085769
B54	0.16(3)	0.04(1)	0.07(2)	-0.01(1)	0.06(2)	0.02(1)
B55	0.04(1)	0.029(9)	0.05(1)	0.014(8)	0.02(1)	0.024(9)
B56	0.16(3)	0.02(1)	0.15(3)	-0.03(1)	0.02(2)	0.01(2)
B57	0.04(1)	0.05(1)	0.16(3)	-0.011(9)	-0.07(1)	0.07(2)

Table S35 Interatomic distances (Å) in the supercell structure of $Ca_2B_2O_5$ at 810 K.

Ca1-O16	2.36(1)	Ca7-O120	3.27(1)	Ca43-O85	2.90(1)	Ca16-O8	2.33(1)	Ca22-O76	3.37(1)	Ca30-O46	2.44(1)
Ca1-O31	2.43(1)	Ca7-O131	3.609(9)	Ca43-O106	3.356(8)	Ca16-O11	2.38(1)	Ca22-O79	2.28(1)	Ca30-O65	2.35(1)
Ca1-O63	2.445(8)	Ca7-O133	2.53(2)	Ca43-O112	2.51(1)	Ca16-O12	2.325(8)	Ca22-O114	3.56(1)	Ca30-O94	2.497(9)
Ca1-O70	2.89(1)	Ca8-O39	2.87(1)	Ca43-O133	3.49(2)	Ca16-O63	2.445(8)	Ca22-O116	2.425(7)	Ca30-O108	3.22(1)
Ca1-O73	2.360(8)	Ca8-O40	2.41(1)	Ca44-O26	2.29(1)	Ca16-O77	2.441(9)	Ca23-O2	2.365(7)	Ca31-O1	2.25(1)
Ca1-O81	2.44(1)	Ca8-O49	2.44(1)	Ca44-O32	2.285(9)	Ca16-O82	2.36(1)	Ca23-O10	2.35(1)	Ca31-O17	3.518(9)
Ca1-O82	2.85(1)	Ca8-O72	2.426(8)	Ca44-O65	2.467(9)	Ca16-O102	3.02(1)	Ca23-O35	2.388(9)	Ca31-O18	2.41(1)
Ca1-O121	3.496(9)	Ca8-O75	2.47(1)	Ca44-O87	2.41(1)	Ca16-O148	3.31(3)	Ca23-O45	2.431(7)	Ca31-O22	2.356(7)
Ca1-O148	2.56(2)	Ca8-O79	2.33(1)	Ca44-O94	3.44(1)	Ca17-O6	2.565(7)	Ca23-O60	3.36(1)	Ca31-O22	3.07(1)
Ca2-O2	3.481(9)	Ca8-O107	3.09(2)	Ca44-O96	2.82(1)	Ca17-O13	2.303(8)	Ca23-O80	2.41(1)	Ca31-O23	2.41(1)
Ca2-O6	2.326(9)	Ca8-O121	2.338(9)	Ca44-O97	2.341(8)	Ca17-O51	2.42(1)	Ca23-O80	2.509(9)	Ca31-O30	2.591(8)
Ca2-O9	2.411(6)	Ca8-O128	3.49(2)	Ca44-O129	2.36(1)	Ca17-O67	2.79(1)	Ca23-O150	3.26(2)	Ca31-O102	2.54(1)
Ca2-O35	2.378(6)	Ca8-O148	3.26(2)	Ca44-O130	3.155(8)	Ca17-O93	2.52(1)	Ca24-O47	2.430(9)	Ca31-O119	3.55(1)
Ca2-O42	2.53(1)	Ca9-O9	2.460(8)	Ca45-O36	2.392(8)	Ca17-O103	2.39(1)	Ca24-O56	2.38(1)	Ca31-O119	3.48(1)
Ca2-O60	2.63(1)	Ca9-O14	2.40(1)	Ca45-O37	2.47(1)	Ca17-O110	2.34(1)	Ca24-O87	2.62(1)	Ca32-O67	2.43(1)

Ca2-O89	2.39(1)	Ca9-O45	2.395(9)	Ca45-O69	2.328(8)	Ca17-O122	3.47(2)	Ca24-O96	2.39(1)	Ca32-O83	2.296(9)
Ca2-O98	2.95(2)	Ca9-O55	2.32(1)	Ca45-O86	2.26(2)	Ca17-O144	3.21(1)	Ca24-O105	2.425(9)	Ca32-O93	3.61(2)
Ca2-O98	3.61(1)	Ca9-O60	2.433(9)	Ca45-O96	3.14(1)	Ca18-O36	2.31(1)	Ca24-O114	3.19(1)	Ca32-O103	3.35(1)
Ca2-O141	3.26(2)	Ca9-O83	2.93(1)	Ca45-O134	3.59(2)	Ca18-O44	3.52(2)	Ca24-O129	3.37(1)	Ca32-O109	2.34(1)
Ca3-O15	2.62(1)	Ca9-O99	3.45(1)	Ca45-O138	2.94(2)	Ca18-O51	2.53(1)	Ca24-O142	2.38(1)	Ca32-O115	2.642(9)
Ca3-O54	3.59(1)	Ca9-O136	2.313(8)	Ca45-O139	2.52(2)	Ca18-O96	2.369(9)	Ca24-O143	3.32(1)	Ca32-O135	2.73(1)
Ca3-O66	2.99(1)	Ca9-O141	2.89(3)	Ca45-O142	2.42(1)	Ca18-O97	2.74(1)	Ca25-O18	2.67(1)	Ca32-O136	2.39(1)
Ca3-O68	2.34(2)	Ca9-O147	3.55(5)	Ca46-O21	2.47(2)	Ca18-O104	3.54(2)	Ca25-O22	2.36(1)	Ca32-O144	2.56(1)
Ca3-O70	2.42(1)	Ca10-O56	2.414(8)	Ca46-O55	2.58(1)	Ca18-O105	2.35(1)	Ca25-O23	2.72(1)	Ca32-O145	3.28(7)
Ca3-O73	2.411(9)	Ca10-O59	2.421(6)	Ca46-O61	2.84(1)	Ca18-O110	2.41(1)	Ca25-O52	2.40(2)	Ca33-O8	2.44(1)
Ca3-O90	2.415(8)	Ca10-O68	2.32(1)	Ca46-O83	2.41(1)	Ca18-O122	2.59(1)	Ca25-O58	2.33(1)	Ca33-O17	2.578(9)
Ca3-O107	3.03(2)	Ca10-O76	2.84(1)	Ca46-O109	2.604(8)	Ca18-O128	3.15(1)	Ca25-O88	2.29(1)	Ca33-O20	2.44(1)
Ca3-O118	2.52(2)	Ca10-O90	2.63(1)	Ca46-O111	2.89(1)	Ca19-O7	2.397(7)	Ca25-O119	2.376(8)	Ca33-O24	2.402(6)
Ca4-O5	2.28(1)	Ca10-O113	3.39(1)	Ca46-O117	2.212(7)	Ca19-O34	2.41(1)	Ca25-O124	2.67(1)	Ca33-O28	2.39(1)
Ca4-O7	3.496(9)	Ca10-O123	2.86(2)	Ca46-O127	2.93(2)	Ca19-O47	3.54(1)	Ca25-O125	3.49(1)	Ca33-O58	3.07(1)
Ca4-O23	2.359(8)	Ca10-O140	3.33(3)	Ca46-O131	2.565(9)	Ca19-O57	2.335(7)	Ca26-O2	2.587(9)	Ca33-O84	3.34(1)
Ca4-O30	2.35(1)	Ca10-O140	2.40(3)	Ca46-O150	3.38(2)	Ca19-O69	2.37(1)	Ca26-O14	3.59(1)	Ca33-O88	2.448(7)
Ca4-O48	2.40(1)	Ca10-O143	2.34(1)	Ca47-O44	2.44(2)	Ca19-O94	2.53(1)	Ca26-O38	2.34(1)	Ca34-O1	2.48(1)
Ca4-O57	2.500(6)	Ca11-O26	2.52(1)	Ca47-O49	2.475(8)	Ca19-O113	3.18(1)	Ca26-O43	2.515(8)	Ca34-O5	2.472(7)
Ca4-O58	2.89(1)	Ca11-O67	2.39(1)	Ca47-O59	2.348(9)	Ca19-O139	3.60(2)	Ca26-O45	2.46(1)	Ca34-O21	2.44(1)
Ca4-O91	2.49(1)	Ca11-O97	2.47(1)	Ca47-O78	2.64(1)	Ca19-O142	2.426(8)	Ca26-O80	2.454(8)	Ca34-O23	3.23(1)
Ca5-O4	2.41(1)	Ca11-O104	2.65(1)	Ca47-O79	3.19(1)	Ca20-O26	2.41(1)	Ca26-O93	3.05(1)	Ca34-O61	2.26(1)
Ca5-O13	2.330(6)	Ca11-O110	2.99(1)	Ca47-O105	2.49(1)	Ca20-O46	2.343(6)	Ca26-O100	2.33(1)	Ca34-O71	3.34(1)
Ca5-O25	2.27(1)	Ca11-O115	2.38(1)	Ca47-O118	3.16(2)	Ca20-O50	2.40(2)	Ca27-O35	2.53(1)	Ca34-O84	2.44(1)
Ca5-O36	2.56(1)	Ca11-O122	3.48(1)	Ca47-O143	2.427(9)	Ca20-O69	2.65(1)	Ca27-O38	2.467(7)	Ca34-O95	2.37(1)
Ca5-O86	2.53(1)	Ca11-O137	2.41(1)	Ca48-O6	2.39(1)	Ca20-O92	3.48(1)	Ca27-O41	3.06(1)	Ca34-O120	3.39(1)
Ca5-O99	3.52(1)	Ca11-O138	3.08(2)	Ca48-O62	2.37(1)	Ca20-O94	2.38(1)	Ca27-O80	3.546(9)	Ca35-O14	2.402(7)
Ca5-O101	3.54(2)	Ca11-O144	3.53(2)	Ca48-O83	3.12(1)	Ca20-O101	3.04(2)	Ca27-O85	2.29(1)	Ca35-O43	2.39(1)
Ca5-O110	2.96(1)	Ca12-O7	2.39(1)	Ca48-O89	3.51(1)	Ca20-O138	2.43(1)	Ca27-O89	2.37(1)	Ca35-O44	2.59(2)
Ca5-O134	2.54(2)	Ca12-O17	2.407(6)	Ca48-O103	2.219(7)	Ca20-O139	3.53(2)	Ca27-O98	2.66(2)	Ca35-O67	3.26(1)
Ca5-O135	3.34(1)	Ca12-O24	2.420(9)	Ca48-O111	2.26(1)	Ca21-O17	2.44(1)	Ca27-O106	3.467(8)	Ca35-O78	2.46(1)
Ca5-O147	3.43(5)	Ca12-O30	2.397(9)	Ca48-O127	3.59(2)	Ca21-O18	2.33(1)	Ca27-O133	3.48(1)	Ca36-O123	2.27(2)
Ca6-O15	2.342(7)	Ca12-O31	2.43(2)	Ca48-O149	2.587(7)	Ca21-O28	2.49(1)	Ca27-O149	2.29(1)	Ca36-O137	2.37(1)
Ca6-O16	2.285(9)	Ca12-O34	2.456(6)	Ca48-O150	2.38(2)	Ca21-O29	2.52(1)	Ca28-O13	2.53(1)	Ca36-O139	3.18(2)
Ca6-O38	2.49(1)	Ca12-O54	3.13(1)	Ca49-O4	2.385(9)	Ca21-O31	2.436(9)	Ca28-O19	3.539(8)	Ca36-O143	2.78(1)
Ca6-O39	3.12(1)	Ca12-O63	3.594(8)	Ca49-O37	2.36(2)	Ca50-O47	2.43(1)	Ca28-O25	2.411(7)	Ca37-O4	2.35(1)
Ca6-O70	2.35(2)	Ca13-O2	2.357(9)	Ca49-O50	2.41(1)	Ca50-O56	2.479(7)	Ca28-O61	3.37(1)	Ca37-O25	2.89(1)
Ca6-O85	2.417(8)	Ca13-O10	2.49(11)	Ca49-O86	3.28(2)	Ca50-O63	2.453(6)	Ca28-O62	2.404(9)	Ca37-O46	2.472(9)
Ca6-O100	3.34(1)	Ca13-O41	2.89(1)	Ca49-O92	2.41(1)	Ca50-O68	2.98(2)	Ca28-O71	2.31(1)	Ca37-O74	2.364(8)
Ca6-	2.39(1	Ca13-	2.39(1	Ca49-	2.69(1	Ca50-	2.40(1	Ca28-	2.45(1	Ca37-	2.389(

O106	)	O42	)	O92	)	O73	)	O74	)	O92	8)
	2.36(1	Ca13-	2.39(1	Ca49-	3.05(1	Ca50-	2.49(1	Ca28-	2.35(1	Ca37-	2.49(2
Ca7-O10	)	O72	)	O104	)	O77	)	O99	)	O108	)
	2.362(	Ca13-	2.30(1	Ca49-	2.44(1	Ca50-	3.359(	Ca28-	2.78(1	Ca37-	3.37(1
Ca7-O41	8)	O75	)	O146	)	O116	6)	O103	)	O130	)
	2.58(1	Ca13-	2.66(1	Ca50-	2.362(		2.53(1	Ca28-	2.87(3	Ca37-	3.29(1
Ca7-O53	)	O100	)	O34	9)	Ca51-O5	)	O141	)	O144	)
	2.376(	Ca13-	3.04(2	Ca14-	2.31(1	Ca51-	2.43(1	Ca29-	2.435(	Ca37-	2.55(8
Ca7-O55	7)	O126	)	O49	)	O19	)	O20	9)	O145	)
	2.39(1		2.43(1	Ca14-	2.35(1	Ca51-	3.28(1	Ca29-	2.57(1	Ca37-	2.56(1
Ca7-O60	)	Ca14-O9	)	O51	)	O25	)	O48	)	O146	)
	2.59(1	Ca14-	2.53(1	Ca14-	3.34(1	Ca51-	2.421(	Ca29-	2.48(1		2.328(
Ca7-O89	)	O14	)	O75	)	O27	7)	O52	)	Ca38-O3	6)
	3.49(1	Ca14-	2.362(	Ca14-	3.29(1	Ca51-	3.49(1	Ca29-	2.39(1	Ca38-	2.48(1
Ca7-O98	)	O42	7)	O106	)	O48	)	O58	)	O32	)
Ca7-	2.62(1	Ca14-	2.36(1	Ca14-	3.11(4	Ca21-	3.06(1	Ca29-	2.82(1	Ca38-	2.29(1
O117	)	O44	)	O147	)	O112	)	O71	)	O33	)
Ca35-	3.28(2	Ca42-	3.61(1		2.388(	Ca21-	2.40(1	Ca29-	2.39(1	Ca38-	3.55(1
O134	)	O77	)	Ca15-O3	9)	O124	)	O74	)	O54	)
Ca35-	2.41(1	Ca42-	3.55(1		2.449(	Ca21-	2.44(1	Ca29-	3.55(2	Ca38-	2.29(1
O136	)	O112	)	Ca15-O8	8)	O125	)	O91	)	O66	)
Ca35-	2.410(	Ca43-	2.56(1	Ca15-	2.43(1	Ca21-	3.268(	Ca29-	2.34(1	Ca38-	3.08(2
O137	8)	O11	)	O47	)	O132	7)	O108	)	O68	)
Ca35-	2.34(5	Ca43-	2.403(	Ca15-	2.44(1	Ca22-	2.36(1	Ca29-	2.85(2	Ca38-	3.41(1
O147	)	O39	7)	O65	)	O33	)	O127	)	O87	)
Ca36-	2.485(	Ca43-	2.33(1	Ca15-	2.44(1	Ca22-	2.448(		2.601(	Ca38-	2.46(1
O32	6)	O41	)	O77	)	O40	7)	Ca30-O7	9)	O113	)
Ca36-	2.404(	Ca43-	2.379(	Ca15-	2.346(	Ca22-	2.477(	Ca30-	3.27(1	Ca38-	2.35(1
O64	8)	O53	9)	O87	8)	O59	8)	O19	)	O123	)
Ca36-	2.354(	Ca43-	2.38(1	Ca15-	3.06(1	Ca22-	3.04(1	Ca30-	2.362(	Ca38-	3.57(2
O78	9)	O72	)	O91	)	O66	)	O20	7)	O140	)
Ca36-	3.28(1	Ca43-	3.29(1	Ca15-	3.39(2	Ca22-	2.330(	Ca30-	2.42(1	Ca39-	2.55(1
O97	)	O82	)	O129	)	O76	8)	O24	)	O27	)

Table S35. (continued).

Ca39-	2.52(1	Ca55-	2.29(1		1.39(	B34-	1.29(		1.34(
O50	)	O15	)	B15-O1	2)	O81	1)	B54-O3	3)
Ca39-	2.78(2	Ca55-	2.38(1	B15-	1.20(	B34-	1.39(	B54-	1.36(
O86	)	O43	)	O17	1)	O119	1)	O24	2)
Ca39-	2.54(2	Ca55-	2.475(	B15-	1.47(	B35-	1.36(	B54-	1.43(
O101	)	O64	7)	O84	2)	O20	1)	O54	4)
Ca39-	2.28(1	Ca55-	2.74(1	B16-	1.41(	B35-	1.44(	B55-	1.48(
O115	)	O75	)	O33	2)	O71	1)	O15	3)
Ca39-	3.18(2	Ca55-	3.53(1	B16-	1.32(	B35-	1.26(	B55-	1.24(
O134	)	O78	)	O87	2)	O84	2)	O78	3)
Ca39-	2.32(1	Ca55-	2.370(	B16-	1.45(	B36-	1.36(	B55-	1.19(
O135	)	O100	9)	O114	2)	O59	1)	O118	4)
Ca39-	2.37(2	Ca55-	2.41(2	B17-	1.29(	B36-	1.33(	B56-	1.14(
O138	)	O107	)	O21	2)	O66	1)	O80	4)
Ca40-	2.48(1	Ca55-	3.33(1	B17-	1.37(	B36-	1.41(		
O12	)	O121	)	O23	1)	O118	3)		
Ca40-	2.44(1	Ca55-	2.97(1	B17-	1.29(		1.37(		
O21	)	O122	)	O119	2)	B37-O4	2)		
Ca40-	2.36(1	Ca55-	2.39(1		1.36(	B37-	1.21(		
O53	)	O128	)	B18-O9	2)	O104	2)		
Ca40-	2.59(1	Ca56-	2.462(	B18-	1.24(	B37-	1.422		
O81	)	O29	7)	O13	2)	O110	)		
Ca40-	2.37(1	Ca56-	2.35(2	B18-	1.70(	B38-	1.29(		
O82	)	O52	)	O99	3)	O88	2)		
Ca40-	3.28(1	Ca56-	2.54(1	B18-	1.40(	B38-	1.55(		
O95	)	O62	)	O141	4)	O124	2)		
Ca40-	2.42(1	Ca56-	2.404(	B19-	1.33(	B38-	1.34(		
O117	)	O71	9)	O41	2)	O125	2)		
Ca40-	3.265(	Ca56-	3.34(1	B19-	1.31(	B38-	1.34(		
O119	8)	O84	)	O42	2)	O132	2)		
Ca40-	3.41(2	Ca56-	2.89(1	B19-	1.42(	B38-	1.49(		
O126	)	O95	)	O98	2)	O132	2)		

Ca40-O131	2.46(1)	Ca56-O111	3.32(1)	B20-O45	1.32(1)	B39-O16	1.41(2)
Ca41-O16	2.466(8)	Ca56-O120	2.43(1)	B20-O83	1.39(1)	B39-O100	1.30(1)
Ca41-O29	2.36(1)	Ca56-O124	2.18(2)	B20-O150	1.34(3)	B39-O126	1.43(3)
Ca41-O81	2.36(1)	Ca56-O125	2.49(2)	B21-O36	1.26(2)	B40-O90	1.33(2)
Ca41-O85	3.06(1)	Ca56-O133	3.15(2)	B21-O44	1.39(2)	B40-O123	1.33(2)
Ca41-O111	2.37(1)	B1-O43	1.49(2)	B21-O134	1.53(3)	B40-O140	1.44(4)
Ca41-O117	3.58(1)	B1-O67	1.20(1)	B21-O147	1.46(6)	B40-O140	1.44(4)
Ca41-O126	2.68(2)	B1-O93	1.32(2)	B22-O32	1.31(1)	B41-O11	1.31(2)
Ca41-O131	2.51(9)	B2-O79	1.44(2)	B22-O94	1.33(2)	B41-O28	1.35(1)
Ca41-O149	2.49(1)	B2-O105	1.31(2)	B22-O113	1.60(2)	B41-O112	1.35(2)
Ca42-O3	2.61(1)	B2-O114	1.36(2)	B23-O62	1.45(2)	B42-O2	1.34(1)
Ca42-O11	2.451(7)	B3-O35	1.43(1)	B23-O89	1.36(1)	B42-O6	1.43(1)
Ca42-O39	2.31(1)	B3-O60	1.30(1)	B23-O120	1.31(2)	B42-O93	1.42(2)
Ca42-O40	2.295(9)	B3-O98	1.28(2)	B23-O133	1.31(3)	B43-O52	1.23(2)
Ca42-O54	2.43(1)	B4-O37	1.30(2)	B24-O73	1.39(2)	B43-O111	1.35(1)
Ca42-O66	2.445(9)	B4-O96	1.37(1)	B24-O107	1.18(2)	B43-O127	1.54(3)
Ca42-O70	3.11(1)	B4-O129	1.42(2)	B24-O121	1.43(2)	B44-O12	1.43(1)
Ca51-O61	2.411(9)	B4-O130	1.44(1)	B24-O148	1.56(2)	B44-O22	1.22(1)
Ca51-O99	3.30(1)	B5-O19	1.50(2)	B25-O51	1.40(2)	B44-O102	1.49(2)
Ca51-O109	2.28(1)	B5-O25	1.31(2)	B25-O75	1.23(2)	B45-O72	1.39(2)
Ca51-O135	2.25(1)	B5-O46	1.29(2)	B25-O122	1.52(2)	B45-O82	1.25(1)
Ca52-O27	2.39(1)	B6-O47	1.32(1)	B25-O128	1.51(3)	B45-O121	1.54(2)
Ca52-O37	2.46(1)	B6-O57	1.37(2)	B26-O55	1.21(1)	B45-O148	1.29(3)
Ca52-O48	2.482(9)	B6-O91	1.48(2)	B26-O61	1.41(1)	B46-O50	1.29(2)
Ca52-O57	2.464(8)	B7-O5	1.31(1)	B26-O99	1.56(2)	B46-O86	1.38(2)
Ca52-O69	3.39(1)	B7-O7	1.42(1)	B26-O141	1.66(3)	B46-O101	1.44(3)
Ca52-O108	2.83(1)	B7-O19	1.39(2)	B27-O26	1.40(2)	B47-O53	1.37(2)
Ca52-O129	3.28(1)	B8-O74	1.26(1)	B27-O92	1.19(2)	B47-O95	1.31(2)
Ca52-O130	2.472(8)	B8-O103	1.41(1)	B27-O104	1.44(2)	B47-O120	1.39(2)
Ca52-O145	3.4(1)	B8-O144	1.39(2)	B28-O48	1.26(1)	B47-O133	1.33(3)
Ca52-O146	2.40(1)	B8-O145	1.80(8)	B28-O109	1.37(2)	B48-O31	1.19(2)
Ca53-O1	2.483(8)	B9-O30	1.20(2)	B28-O127	1.36(3)	B48-O54	1.45(2)
Ca53-O12	2.47(1)	B9-O63	1.43(1)	B29-O8	1.32(2)	B48-O70	1.47(2)
Ca53-O22	2.88(1)	B9-O102	1.43(2)	B29-O58	1.36(1)	B49-O134	1.17(5)
Ca53-O28	2.468(7)	B10-O39	1.32(2)	B29-O91	1.39(2)	B49-O135	1.60(4)
Ca53-O88	2.53(1)	B10-O49	1.37(2)	B30-O27	1.38(1)	B49-O136	1.40(4)
Ca53-O95	2.35(1)	B10-O106	1.39(2)	B30-O69	1.28(1)	B49-O147	1.39(8)
Ca53-O124	3.53(1)	B11-O40	1.33(2)	B30-O101	1.42(3)	B50-O137	1.46(2)
Ca53-O125	2.62(1)	B11-O77	1.31(1)	B31-O34	1.34(1)	B50-O138	1.32(3)
Ca53-	2.41(1	B11-	1.53(1	B31-	1.30(	B50-	1.29(

O132	)	O116	)	O68	2)	O139	3)
Ca53-O132	3.39(1)	B12-O14	1.37(1)	B31-O113	1.33(2)	B51-O56	1.49(5)
Ca54-O33	2.56(1)	B12-O38	1.34(1)	B32-O10	1.33(2)	B51-O76	1.20(4)
Ca54-O64	2.477(9)	B12-O106	1.49(1)	B32-O117	1.41(2)	B51-O116	1.32(6)
Ca54-O76	2.38(1)	B13-O64	1.38(3)	B32-O126	1.35(3)	B52-O139	1.34(4)
Ca54-O79	3.01(1)	B13-O97	1.36(2)	B32-O131	1.28(2)	B52-O142	1.40(3)
Ca54-O90	2.32(1)	B13-O122	1.34(3)	B33-O65	1.36(2)	B52-O143	1.23(3)
Ca54-O107	2.36(1)	B13-O128	1.36(3)	B33-O108	1.26(2)	B53-O115	1.33(3)
Ca54-O114	2.44(1)	B14-O29	1.50(1)	B33-O129	1.43(2)	B53-O144	1.36(3)
Ca54-O116	3.357(8)	B14-O85	1.18(2)	B33-O130	1.33(2)	B53-O145	0.9(1)
Ca54-O123	3.29(2)	B14-O112	1.41(2)	B34-O18	1.43(2)	B53-O146	1.47(2)

Table S36 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 830 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7648(1)	–0.40121(8)	0.14426(5)	0.0331(2)
O1	1	0.7490(4)	0.8286(3)	0.4022(2)	0.0639(9)
O2	1	0.7512(5)	0.4058(3)	0.3297(2)	0.0445(6)
O3	0.5	0.482(2)	0.077(1)	–0.0138(6)	0.049(2)
B1	1	0.6775(6)	0.5821(4)	0.4079(2)	0.0238(7)

Table S37 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 830 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0233(3)	0.0255(3)	0.0503(4)	0	0.0006(2)	0.0091(2)
O1	0.034(1)	0.0209(8)	0.136(2)	0	0	0.001(1)
O2	0.050(1)	0.045(1)	0.039(1)	0.0167(8)	0	0
O3	0.071(2)	0.044(3)	0.033(4)	0.019(4)	0.022(2)	0.010(3)
B1	0.021(1)	0.026(1)	0.024(1)	0.0019(9)	0	0.002(1)

Table S38 Occupational and displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 830 K.

Atom	SOF	Wave	*x*	*y*	*z*
Ca1	1	s,1,0	–0.0043(3)	0.00454(2)	0.00461(9)
	1	c,1,0	–0.0053(3)	0.0087(2)	0.00570(8)
	1	s,0,1	–0.0032(2)	0.0037(2)	0.00959(8)
	1	c,0,1	0.0011(3)	0.0008(2)	0.00516(8)
O1	1	s,1,0	–0.0062(8)	–0.0046(5)	0.0092(3)
	1	c,1,0	0.000(1)	–0.0001(5)	–0.0019(3)
	1	s,0,1	0.0101(8)	–0.0008(5)	–0.0139(3)
	1	c,0,1	0.0130(9)	0.0084(5)	–0.0199(3)
O2	1	s,1,0	–0.0142(9)	0.0006(5)	0.0008(3)
	1	c,1,0	–0.0012(8)	0.0031(5)	0.0045(2)
	1	s,0,1	–0.0218(8)	–0.0189(5)	0.0123(2)
	1	c,0,1	–0.0012(9)	0.0051(5)	0.0009(3)
O3	0.5	s,1,0	–0.004(2)	–0.014(3)	–0.0006(8)
	0.5	c,1,0	0.014(2)	–0.001(1)	–0.0013(7)
	0.5	s,0,1	–0.013(2)	0.002(2)	0.0061(7)
	0.5	c,0,1	–0.008(2)	0.011(1)	–0.0013(6)
B1	1	s,1,0	–0.004(1)	0.0053(4)	–0.012(1)
	1	c,1,0	0.000(1)	0.0030(4)	0.003(1)
	1	s,0,1	0.007(1)	–0.0011(4)	–0.001(1)
	1	c,0,1	0.0088(9)	–0.0002(4)	–0.000(1)

Table S39 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 830 K.

Ato	Wav	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}

m	e						
Ca1	s,1,0	–0.0007(6)	–0.0023(5)	0.0063(7)	0.0006(4)	–0.0006(5)	0.0003(4)
	c,1,0	0.0002(6)	–0.0018(5)	0.0103(7)	0.0014(5)	–0.0002(5)	0.0034(5)
	s,0,1	–0.0008(6)	–0.0015(5)	–0.0028(7)	0.0006(4)	0.0006(5)	–0.0001(4)
	c,0,1	–0.0007(6)	0.0024(5)	0.0126(7)	–0.0008(4)	–0.0017(5)	0.0046(5)
O1	s,1,0	0.001(3)	–0.001(2)	0.015(4)	0.001(2)	–0.004(2)	–0.006(2)
	c,1,0	0.003(2)	–0.001(2)	0.058(4)	–0.001(2)	–0.010(2)	0.000(2)
O2	s,1,0	–0.009(2)	–0.008(2)	–0.002(2)	–0.009(1)	0.004(1)	0.003(1)
	c,1,0	0.007(2)	0.004(2)	0.005(2)	0.008(2)	–0.002(1)	–0.004(1)
	s,0,1	–0.003(2)	–0.001(2)	0.004(2)	–0.002(1)	–0.003(1)	–0.003(1)
	c,0,1	0.007(2)	0.006(2)	0.007(2)	0.006(1)	–0.004(1)	–0.006(1)
O3	s,1,0	0	0	0.001(7)	0.008(5)	0	0.007(5)
	c,1,0	0.000(5)	0	0.000(5)	0	0.000(4)	0.003(4)
	s,0,1	0.004(6)	–0.003(7)	0	0.002(3)	0.004(4)	0
	c,0,1	0	0	0	0	0	0.005(4)
B1	s,1,0	–0.002(3)	0.003(3)	–0.002(3)	0.005(2)	–0.001(2)	–0.001(2)
	c,1,0	–0.001(3)	–0.008(3)	0.005(3)	0.004(2)	0.000(2)	0.000(2)
	s,0,1	–0.001(3)	–0.004(3)	–0.001(3)	–0.002(2)	–0.003(2)	–0.004(2)
	c,0,1	–0.003(3)	0.002(3)	–0.002(3)	0.000(2)	–0.002(2)	0.000(2)

Table S40 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 830 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.393(7)	2.366(7)	2.436(7)
Ca1–O1(ii)	2.347(7)	2.271(7)	2.424(7)
Ca1–O1(iii)	2.835(8)	2.377(8)	3.308(8)
Ca1–O2(iv)	2.386(6)	2.294(6)	2.468(6)
Ca1–O2(v)	2.497(6)	2.394(7)	2.607(7)
Ca1–O2(vi)	2.396(6)	2.349(6)	2.436(6)
Ca1–O3(vii)	2.42(2)	2.39(2)	2.47(2)
B1–O1	1.33(1)	1.29(1)	1.37(1)
B1–O2	1.34(1)	1.31(1)	1.38(1)
B1–O3(viii)	1.38(2)	1.33(2)	1.44(2)
B1–O3(ix)	1.44(2)	1.40(2)	1.49(2)

Symmetry codes: (i) *–x+1, y–3/2, –z+1/2*; (ii) *–x+2, y–3/2, –z+1/2*; (iii) *x, –y+1/2, z–1/2*; (iv) *x, y–1, z*; (v) *–x+1, y–1/2, –z+1/2*; (vi) *–x+2, y–1/2, –z+1/2*; (vii) *–x+1, –y, –z*; (viii) *–x+1, y+1/2, –z+1/2*; (ix) *x, –y+1/2, z+1/2*.

Table S41 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 840 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.76474(1)	–0.40109(8)	0.14407(5)	0.0333(2)
O1	1	0.7495(4)	0.8281(3)	0.4026(2)	0.0675(9)
O2	1	0.7502(5)	0.4062(3)	0.3295(2)	0.0454(7)
O3	0.5	0.482(2)	0.077(1)	–0.0127(6)	0.053(2)
B1	1	0.6779(6)	0.5825(4)	0.4078(2)	0.0240(7)

Table S42 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 840 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0236(3)	0.0263(3)	0.0498(4)	0	0.0001(2)	0.0094(2)
O1	0.036(1)	0.0229(9)	0.143(2)	0	0	0
O2	0.050(1)	0.045(1)	0.041(1)	0.0154(8)	0	0
O3	0.076(3)	0.044(3)	0.039(4)	0.018(3)	0.024(2)	0.004(3)
B1	0.022(1)	0.026(1)	0.024(1)	0.0023(9)	0	0.0018(9)

Table S43 Occupational and displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 840 K.

Atom	SOF	Wave	*x*	*y*	*z*
Ca1	1	s,1,0	–0.0040(2)	0.0039(2)	0.00425(8)
	1	c,1,0	–0.0055(2)	0.0080(1)	0.00536(7)
	1	s,0,1	–0.0034(2)	0.0038(1)	0.00899(7)
	1	c,0,1	0.0005(2)	0.0008(1)	0.00497(7)
O1	1	s,1,0	–0.0065(7)	–0.0040(5)	0.0095(3)
	1	c,1,0	–0.0001(8)	0.0006(5)	–0.0019(3)

	1	s,0,1	0.0081(8)	–0.0013(5)	–0.0125(3)
	1	c,0,1	0.0122(8)	0.0076(5)	–0.0183(3)
O2	1	s,1,0	–0.0124(8)	0.0008(5)	0.0007(2)
	1	c,1,0	–0.0022(7)	0.0029(5)	0.0043(2)
	1	s,0,1	–0.0210(7)	–0.0170(5)	0.0117(2)
	1	c,0,1	–0.0008(8)	0.0045(5)	0.0011(2)
O3	0.5	s,1,0	0.000(2)	–0.012(3)	0.0007(8)
	0.5	c,1,0	0.013(2)	0.001(1)	–0.0007(6)
	0.5	s,0,1	–0.013(2)	0.003(2)	0.0053(5)
	0.5	c,0,1	–0.007(2)	0.010(1)	–0.0013(6)
B1	1	s,1,0	–0.0032(9)	0.0060(4)	–0.011(1)
	1	c,1,0	0.0008(9)	0.0028(4)	0.002(1)
	1	s,0,1	0.0059(9)	–0.0016(4)	–0.005(1)
	1	c,0,1	0.0066(8)	–0.0007(4)	0.000(1)

Table S44 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 840 K.

Atom	Wave	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1,0	–0.0006(5)	–0.0013(5)	0.0058(6)	0.0003(4)	–0.0005(4)	0.0011(4)
	c,1,0	–0.0003(5)	–0.0019(5)	0.0098(6)	0.0008(4)	–0.0004(4)	0.0033(4)
	s,0,1	–0.0008(5)	–0.0012(5)	–0.0022(6)	0.0007(4)	0.0002(4)	–0.0001(4)
	c,0,1	0.0001(5)	0.0017(5)	0.0102(6)	–0.0003(4)	–0.0014(4)	0.0042(4)
O1	s,1,0	0.000(2)	0.000(2)	0.012(4)	0.002(2)	–0.004(2)	–0.002(2)
	c,1,0	0.001(2)	–0.002(2)	0.058(4)	–0.001(2)	–0.011(2)	0.001(2)
O2	s,1,0	–0.005(2)	–0.003(2)	–0.003(2)	–0.007(2)	0.004(2)	0.003(2)
	c,1,0	0.009(2)	0.001(2)	0.005(2)	0.007(2)	0.000(2)	–0.002(2)
	s,0,1	–0.007(2)	–0.004(2)	0.006(2)	–0.003(2)	–0.003(1)	–0.004(1)
	c,0,1	0.008(2)	0.003(2)	0.005(2)	0.005(2)	–0.002(2)	–0.005(2)
O3	s,1,0	0	0	0.013(6)	0.007(5)	0	–0.001(5)
	c,1,0	0.003(5)	–0.003(6)	0.004(4)	0	0.001(3)	0
	s,0,1	0	0	0	0.000(3)	0	–0.003(3)
	c,0,1	–0.002(5)	0	0	0	0.001(3)	0.004(4)
B1	s,1,0	0.000(3)	0.002(3)	–0.001(2)	0.003(2)	0.000(2)	–0.003(2)
	c,1,0	0.002(3)	–0.004(3)	0.000(3)	0.000(2)	–0.001(2)	0.000(2)
	s,0,1	–0.002(3)	–0.003(3)	0.001(3)	0.000(2)	–0.004(2)	–0.003(2)
	c,0,1	–0.001(3)	0.000(3)	0.003(3)	–0.001(2)	–0.003(2)	0.002(2)

Table S45 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 840 K.

Bond	Average	Min.	Max.
Ca1–O1(i)	2.395(6)	2.368(6)	2.438(6)
Ca1–O1(ii)	2.347(6)	2.280(6)	2.417(6)
Ca1–O1(iii)	2.828(8)	2.397(8)	3.271(8)
Ca1–O2(iv)	2.384(6)	2.297(6)	2.462(6)
Ca1–O2(v)	2.495(6)	2.397(6)	2.604(6)
Ca1–O2(vi)	2.399(6)	2.358(6)	2.434(6)
Ca1–O3(vii)	2.43(2)	2.38(2)	2.48(2)
B1–O1	1.32(1)	1.29(1)	1.37(1)
B1–O2	1.34(1)	1.30(1)	1.39(1)
B1–O3(viii)	1.37(2)	1.32(2)	1.42(2)
B1–O3(ix)	1.43(2)	1.48(2)	1.45(2)

Symmetry codes: (i) *–x+1, y–3/2, –z+1/2*; (ii) *–x+2, y–3/2, –z+1/2*; (iii) *x, –y+1/2, z–1/2*; (iv) *x, y–1, z*; (v) *–x+1, y–1/2, –z+1/2*; (vi) *–x+2, y–1/2, –z+1/2*; (vii) *–x+1, –y, –z*; (viii) *–x+1, y+1/2, –z+1/2*; (ix) *x, –y+1/2, z+1/2*.

Table S46 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 850 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7647(1)	–0.40086(8)	0.14387(5)	0.0347(2)
O1	1	0.7483(4)	0.8293(3)	0.4029(2)	0.073(1)
O2	1	0.7521(5)	0.4066(3)	0.3293(2)	0.0478(7)
O3	0.5	0.480(2)	0.0781(8)	–0.0124(5)	0.051(2)
B1	1	0.6790(6)	0.5828(4)	0.4075(2)	0.0249(7)

Table S47 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 850 K.

Ato	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}

m						
Ca1	0.0240(3)	0.0267(3)	0.0534(4)	0	0.0003(2)	0.0100(2)
O1	0.036(1)	0.0233(9)	0.157(3)	0	0	0
O2	0.054(1)	0.046(1)	0.043(1)	0.0180(8)	0	0
O3	0.074(3)	0.042(2)	0.038(3)	0.022(3)	0.021(2)	0.003(2)
B1	0.021(1)	0.026(1)	0.027(1)	0.0015(9)	0	0.001(1)

Table S48 Occupational and displacive modulation wave parameters of atoms in the structure of $Ca_2B_2O_5$ at 850 K.

Atom	SOF	Wave	*x*	*y*	*z*
Ca1	1	s,1,0	–0.0033(3)	0.0030(2)	0.0031(1)
	1	c,1,0	–0.0052(3)	0.0059(2)	0.00387(9)
	1	s,0,1	–0.0033(3)	0.0027(2)	0.0070(1)
	1	c,0,1	0.0003(3)	0.0008(2)	0.0039(1)
O1	1	s,1,0	–0.006(1)	–0.0036(7)	0.0077(4)
	1	c,1,0	0.001(1)	0.0008(6)	–0.0024(4)
	1	s,0,1	0.008(1)	–0.0006(6)	–0.0101(4)
	1	c,0,1	0.010(1)	0.0057(7)	–0.0142(4)
O2	1	s,1,0	–0.008(1)	0.0007(7)	0.0009(3)
	1	c,1,0	–0.000(1)	0.0026(6)	0.0036(3)
	1	s,0,1	–0.017(1)	–0.0133(6)	0.0094(3)
	1	c,0,1	–0.001(1)	0.0032(6)	0.0010(3)
O3	0.5	s,1,0	–0.005(2)	–0.009(3)	0.0016(7)
	0.5	c,1,0	0.002(3)	–0.001(1)	–0.0009(7)
	0.5	s,0,1	–0.012(2)	0.003(2)	0.0043(6)
	0.5	c,0,1	–0.007(2)	0.006(1)	–0.0007(7)
B1	1	s,1,0	–0.010(2)	–0.002(1)	0.0051(5)
	1	c,1,0	0.002(2)	0.001(1)	0.0020(5)
	1	s,0,1	–0.005(2)	0.005(1)	–0.0007(5)
	1	c,0,1	0.001(2)	0.005(1)	0.0003(5)

Table S49 Modulation of anisotropic parameters of atoms (Å^2) in the structure of $Ca_2B_2O_5$ at 850 K.

Atom		U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	s,1,0	–0.0013(7)	–0.0013(6)	0.0048(8)	0.0003(5)	–0.0012(6)	0.0014(5)
	c,1,0	–0.0005(7)	–0.0026(7)	0.0083(9)	0.0007(6)	0.0010(6)	0.0021(6)
	s,0,1	–0.0010(7)	–0.0015(7)	–0.0006(8)	0.0003(5)	0.0006(6)	–0.0002(5)
	c,0,1	–0.0002(7)	0.0006(6)	0.0100(8)	–0.0006(5)	–0.0006(6)	0.0034(6)
O1	s,1,0	0.001(3)	0.000(2)	0.003(5)	0.004(2)	0.000(3)	–0.006(3)
	c,1,0	–0.001(3)	–0.002(2)	0.046(5)	0.002(2)	–0.005(3)	0.000(3)
O2	s,1,0	–0.007(3)	–0.003(2)	–0.002(3)	–0.004(2)	0.002(2)	0.001(2)
	c,1,0	0.007(3)	0.006(3)	–0.001(3)	0.008(2)	0.000(2)	0.001(2)
	s,0,1	–0.007(3)	–0.003(2)	0.005(2)	–0.002(2)	–0.003(2)	–0.008(2)
	c,0,1	0.005(3)	0.000(2)	0.009(3)	0.006(2)	–0.004(2)	–0.003(2)
O3	s,1,0	0	0	0.009(7)	0.016(5)	0	0
	c,1,0	0	0	0.006(5)	0.017(6)	0	0
	s,0,1	0	0	0.003(5)	0	0	0
	c,0,1	0	0	0	0	0	0.006(5)
B1	s,1,0	0.000(4)	0.004(4)	–0.002(3)	0.004(3)	0.001(3)	–0.006(3)
	c,1,0	0.007(4)	–0.003(4)	–0.004(4)	0.003(3)	0.004(3)	0.003(3)
	s,0,1	0.000(4)	–0.007(4)	0.004(4)	0.001(3)	–0.005(3)	–0.005(3)
	c,0,1	–0.008(4)	0.002(4)	0.004(4)	–0.005(3)	–0.003(3)	0.001(3)

Table S50 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 850 K.

	Average	Min.	Max.
Ca1–O1(i)	2.388(8)	2.366(8)	2.420(8)
Ca1–O1(ii)	2.347(8)	2.288(8)	2.408(8)
Ca1–O1(iii)	2.82(1)	2.48(1)	3.17(1)
Ca1–O2(iv)	2.380(7)	2.316(8)	2.438(8)
Ca1–O2(v)	2.502(8)	2.427(8)	2.585(8)
Ca1–O2(vi)	2.395(8)	2.366(8)	2.417(8)
Ca1–O3(vii)	2.419(2)	2.37(2)	2.46(2)
B1–O1	1.33(1)	1.30(1)	1.37(1)
B1–O2	1.37(2)	1.33(2)	1.41(2)
B1–O3(viii)	1.33(2)	1.41(2)	1.37(2)

B1–O3(ix)	1.45(2)	1.48(2)	1.47(2)

Symmetry codes: (i) *–x+1, y–3/2, –z+1/2*; (ii) *–x+2, y–3/2, –z+1/2*; (iii) *x, –y+1/2, z–1/2*; (iv) *x, y–1, z*; (v) *–x+1, y–1/2, –z+1/2*; (vi) *–x+2, y–1/2, –z+1/2*; (vii) *–x+1, –y, –z*; (viii) *–x+1, y+1/2, –z+1/2*; (ix) *x, –y+1/2, z+1/2*.

Table S51 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 900 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7652(2)	–0.4002(2)	0.14329(9)	0.0375(4)
O1	1	0.750(1)	0.8303(7)	0.4042(5)	0.082(2)
O2	1	0.751(1)	0.4074(6)	0.3281(3)	0.054(1)
O3	0.5	0.474(3)	0.075(1)	–0.0129(8)	0.062(4)
B1	1	0.677(1)	0.5836(8)	0.4077(4)	0.027(1)

Table S52 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 900 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0249(6)	0.0283(6)	0.0592(8)	0	0.0017(4)	0.0110(4)
O1	0.040(2)	0.023(2)	0.181(6)	0	0	0
O2	0.057(3)	0.052(2)	0.051(2)	0.020(2)	0	0
O3	0.082(6)	0.058(6)	0.049(5)	0.033(5)	0.030(5)	0.010(5)
B1	0.024(2)	0.027(3)	0.029(3)	0.002(2)	0.001(2)	0.001(2)

Table S53 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 900 K.

Ca1–O1(i)	2.391(4)
Ca1–O1(ii)	2.339(4)
Ca1–O2(iii)	2.369(4)
Ca1–O2(iv)	2.395(4)
Ca1–O3(v)	2.409(9)
B1–O1	1.316(6)
B1–O2	1.342(7)
B1–O3	1.36(1)
B1–O3(vi)	1.46(1)

Symmetry codes: (i) *–x+1, –y–3/2, –z+1/2*; (ii) *–x+2, y–3/2, –z+1/2*; (iii) *x, y–1, z*; (iv) *–x+2, y–1/2, –z+1/2*; (v) *–x+1, –y, –z*; (vi) *–x+1, y+1/2, –z+1/2*; (vi) *x, –y+1/2, z+1/2*; (vi) *x, –y+1/2, z+1/2*.

Table S54 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 1000 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7656(3)	–0.3994(2)	0.1428(1)	0.0395(4)
O1	1	0.748(1)	0.8298(7)	0.4056(5)	0.080(2)
O2	1	0.752(1)	0.4103(7)	0.3278(3)	0.056(2)
O3	0.5	0.474(4)	0.070(2)	–0.014(1)	0.064(4)
B1	1	0.677(2)	0.582(1)	0.4082(5)	0.030(2)

Table S55 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 1000 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0300(6)	0.0325(6)	0.0558(8)	–0.0010(4)	–0.0016(5)	0.0102(5)
O1	0.041(3)	0.031(2)	0.167(6)	–0.004(2)	–0.021(3)	–0.002(3)
O2	0.062(3)	0.057(3)	0.048(3)	0.018(2)	–0.007(2)	–0.020(2)
O3	0.088(7)	0.070(9)	0.035(6)	0.043(7)	0.020(5)	0.010(6)
B1	0.025(3)	0.033(3)	0.031(3)	0.003(2)	–0.002(2)	0.002(3)

Table S56 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 1000 K.

Ca1–O1(i)	2.402(4)
Ca1–O1(ii)	2.357(4)
Ca1–O2(iii)	2.365(4)
Ca1–O2(iv)	2.409(4)
Ca1–O3(v)	2.42(1)
B1–O1	1.321(7)
B1–O2	1.329(7)

B1–O3(vii) 1.364(1)
B1–O3(vii) 1.43(1)

Symmetry codes: (i) –*x*+1, –*y*–3/2, –*z*+1/2; (ii) –*x*+2, *y*–3/2, –*z*+1/2; (iii) *x*, *y*–1, *z*; (iv) –*x*+2, *y*–1/2, –*z*+1/2; (v) –*x*+1, –*y*, –*z*; (vi) –*x*+1, *y*+1/2, –*z*+1/2; (vi) *x*, –*y*+1/2, *z*+1/2.

Table S57 Atomic site occupancy factors (SOF), coordinates and displacement parameters (Å^2) in the structure of $Ca_2B_2O_5$ at 1100 K.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Ca1	1	0.7659(2)	–0.3990(1)	0.14249(8)	0.0402(3)
O1	1	0.7492(7)	0.8321(5)	0.4052(4)	0.080(2)
O2	1	0.7507(8)	0.4090(5)	0.3283(3)	0.056(1)
O3	0.5	0.481(3)	0.071(1)	–0.0124(8)	0.068(3)
B1	1	0.678(1)	0.5848(7)	0.4077(4)	0.030(1)

Table S58 Anisotropic parameters of atomic displacements (Å^2) in the structure of $Ca_2B_2O_5$ at 1100 K.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ca1	0.0305(5)	0.0331(5)	0.0571(6)	0	0.0016(3)	0.0091(4)
O1	0.045(2)	0.027(2)	0.166(4)	0	0	0
O2	0.064(2)	0.056(2)	0.049(2)	0.019(1)	0	0
O3	0.102(5)	0.060(6)	0.044(5)	0.030(5)	0.035(4)	0.011(5)
B1	0.028(2)	0.030(2)	0.032(2)	0.003(2)	0.002(2)	0.005(2)

Table S59 Interatomic distances (Å) in the structure of $Ca_2B_2O_5$ at 1100 K.

Ca1–O1(i) 2.402(3)
Ca1–O1(ii) 2.349(3)
Ca1–O2(iii) 2.380(3)
Ca1–O2(iv) 2.409(3)
Ca1–O3(v) 2.435(8)
B1–O1 1.317(5)
B1–O2 1.335(5)
B1–O3(vi) 1.37(1)
B1–O3(vii) 1.45(1)

Symmetry codes: (i) –*x*+1, –*y*–3/2, –*z*+1/2; (ii) –*x*+2, *y*–3/2, –*z*+1/2; (iii) *x*, *y*–1, *z*; (iv) –*x*+2, *y*–1/2, –*z*+1/2; (v) –*x*+1, –*y*, –*z*; (vi) –*x*+1, *y*+1/2, –*z*+1/2; (vi) *x*, –*y*+1/2, *z*+1/2.

References

1 I. Kusachi, S. Kobayashi, Y. Takechi, Y. Nakamuta, T. Nagase, K. Yokoyama, K. Momma, R. Miyawaki, M. Shigeoka and S. Matsubara, *Mineral. Mag*., 2013, **77**, 93–105. DOI: 10.1180/minmag.2013.077.1.09.
2 C. Heyward, *All Dissertations*, 2013, 1164.
3 K. K. Kelley, Critical Evaluation of High Temperature Heat Capacities of Inorganic Compounds, US. Bur. Mines, Bull., 1949.
4 V. Yukhno, S. Volkov, R. Bubnova, A. Povolotskiy and V. Ugolkov*, Solid State Sci*., 2021, **121**, 106726. DOI: 10.1016/j.solidstatesciences.2021.106726.
5 H. Witzmann and W. Beulich, *Z. Phys. Chem*., 1964, **225**, 336–341.
6 S. Volkov, M. Dušek, R. Bubnova, M. Krzhizhanovskaya, V. Ugolkov, E. Obozova and S. Filatov, *Acta Crystallogr. B*, 2017, **73**, 1056–1067. DOI: 10.1107/S2052520617012689.