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Supporting information for article:

Variation of cation distribution with temperature and its consequences on thermal expansion for Ca3Eu2(BO3)4

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Table S1 Foreign peaks at the diffractogram of $Ca_3Eu_2(BO_3)_4$ at 295 K.

2θ position [°]	***d* [Å]**	**Intensity (I_{max} ~35080) [counts]**
2.86	8.019	15
3.19	7.189	20
3.23	7.100	20
4.15	5.527	40
7.44	3.084	120
10.14	2.264	35

Table S2 Lattice constants for $Ca_3Eu_2(BO_3)_4$ versus temperature.

***T* [K]**	***a* [Å]**	***b* [Å]**	***c* [Å]**
295	7.20378(2)	15.57492(5)	8.63406(3)
323	7.20569(2)	15.57838(5)	8.63488(3)
373	7.21013(2)	15.58993(5)	8.63861(3)
423	7.21468(2)	15.60259(5)	8.64275(3)
473	7.21910(2)	15.61557(5)	8.64690(3)
523	7.22380(2)	15.62922(5)	8.65125(3)
573	7.22857(2)	15.64299(5)	8.65529(3)
623	7.23366(2)	15.65736(5)	8.65935(3)
673	7.23882(2)	15.67186(5)	8.66320(3)
723	7.24415(2)	15.68668(5)	8.66692(3)
773	7.24966(2)	15.70092(5)	8.67029(3)
823	7.25581(2)	15.71408(5)	8.67338(3)
873	7.26226(2)	15.72632(5)	8.67618(2)
923	7.26798(2)	15.74181(4)	8.67958(2)
973	7.27031(2)	15.76770(4)	8.68347(2)
1023	7.27230(2)	15.79486(4)	8.68703(2)
1073	7.27449(2)	15.82021(4)	8.69040(2)
1123	7.27737(2)	15.84377(4)	8.69354(2)
1173	7.28092(2)	15.86528(4)	8.69633(2)

Table S3 Eu occupation in cationic sites for $Ca_3Eu_2(BO_3)_4$ versus temperature.

***T* [K]**	**M1**	**M3**	**M3**
295	0.469(1)	0.260(1)	0.543(2)
323	0.468(1)	0.260(1)	0.544(2)
373	0.468(1)	0.260(1)	0.543(2)
423	0.469(1)	0.260(1)	0.543(2)
473	0.4692(9)	0.258(1)	0.545(2)
523	0.4689(9)	0.260(1)	0.543(2)
573	0.4683(9)	0.261(1)	0.542(2)

623	0.4687(9)	0.262(1)	0.539(2)
673	0.4697(9)	0.260(1)	0.540(2)
723	0.4701(9)	0.260(1)	0.539(2)
773	0.4705(9)	0.260(1)	0.540(2)
823	0.4733(9)	0.256(1)	0.541(1)
873	0.4745(8)	0.254(1)	0.544(1)
923	0.4740(8)	0.254(1)	0.544(1)
973	0.4738(8)	0.262(1)	0.529(1)
1023	0.4717(8)	0.269(1)	0.519(1)
1073	0.4714(8)	0.274(1)	0.509(1)
1123	0.4708(9)	0.279(1)	0.501(1)
1173	0.4699(9)	0.285(1)	0.490(2)

Table S4 Isotropic thermal displacement parameters for Ca/RE, B and O atoms in $Ca_3Eu_2(BO_3)_4$ structure versus temperature.

T **[K]**	**Ca/RE** B_{iso}**[Å²]**	**B** B_{iso}**[Å²]**	**O** B_{iso}**[Å²]**
295	1.69(2)	6.0(4)	4.5(1)
323	1.70(2)	5.9(4)	4.6(1)
373	1.77(2)	6.0(4)	4.7(1)
423	1.84(2)	6.2(4)	4.8(1)
473	1.91(2)	6.3(4)	4.8(1)
523	1.92(2)	6.2(4)	4.8(1)
573	2.05(2)	5.9(4)	4.9(1)
623	2.13(2)	6.2(4)	5.0(1)
673	2.19(2)	6.5(4)	5.1(1)
723	2.20(2)	6.6(4)	5.2(1)
773	2.36(2)	6.7(4)	5.2(1)
823	2.36(2)	6.7(4)	5.2(1)
873	2.54(2)	6.4(4)	5.5(1)
923	2.63(2)	6.4(4)	5.5(1)
973	2.63(2)	6.4(4)	5.5(1)
1023	2.67(2)	7.8(4)	5.7(1)
1073	2.71(2)	8.4(4)	5.8(1)
1123	2.78(2)	8.0(4)	5.8(1)
1173	2.92(2)	9.8(5)	5.9(1)

Table S5 R_{wp} factors for Rietveld refinement of $Ca_3Eu_2(BO_3)_4$ structure versus temperature.

T [K]	R_{wp} [%]
295	9.1
323	9.4
373	9.3
423	9.3
473	9.2
523	9.0
573	8.9
623	8.9
673	8.7
723	8.7
773	8.5
823	8.4
873	8.2
923	8.2
973	8.0
1023	8.1
1073	8.3
1123	8.3
1173	8.4

Table S6 Atomic coordinates of $Ca_3Eu_2(BO_3)_4$ structure versus temperature (part 1).

T [K]	M1x	M1y	M1z	M2x	M2y	M2z	M3x	M3z	B1x	B1y	B1z	B2x	B2z	B3x	B3z
295	0.51946(14)	0.08348(6)	0.82354(12)	0.69687(19)	0.12768(8)	0.34419(16)	0.32762(18)	0.53358(15)	0.3334(27)	0.4488(11)	0.4466(21)	0.7100(34)	0.6552(30)	0.4898(36)	0.1335(28)
323	0.51945(14)	0.08347(7)	0.82352(12)	0.69689(20)	0.12767(8)	0.34417(16)	0.32766(19)	0.53358(16)	0.3334(28)	0.4488(11)	0.4466(22)	0.7102(35)	0.6552(31)	0.4901(37)	0.1333(29)
373	0.51949(15)	0.08345(7)	0.82338(12)	0.69681(20)	0.12767(8)	0.34425(16)	0.32756(19)	0.53345(16)	0.3333(28)	0.4487(11)	0.4467(21)	0.7102(35)	0.6552(30)	0.4901(37)	0.1336(29)
423	0.51960(15)	0.08343(7)	0.82337(12)	0.69661(20)	0.12769(8)	0.34457(16)	0.32722(19)	0.53331(16)	0.3331(28)	0.4486(12)	0.4467(21)	0.7098(35)	0.6554(30)	0.4899(38)	0.1340(29)
473	0.51963(15)	0.08343(7)	0.82321(13)	0.69658(20)	0.12773(8)	0.34476(16)	0.32702(19)	0.53295(16)	0.3331(28)	0.4485(11)	0.4468(21)	0.7095(35)	0.6554(30)	0.4900(38)	0.1339(29)
523	0.51963(14)	0.08343(6)	0.82320(12)	0.69655(19)	0.12773(8)	0.34479(16)	0.32699(18)	0.53293(16)	0.3330(27)	0.4486(11)	0.4468(21)	0.7095(35)	0.6555(30)	0.4900(37)	0.1340(29)
573	0.51968(15)	0.08344(6)	0.82298(12)	0.69629(19)	0.12769(8)	0.34525(16)	0.32659(18)	0.53262(16)	0.3329(26)	0.4484(11)	0.4467(20)	0.7107(34)	0.6559(29)	0.4897(36)	0.1346(28)
623	0.51967(15)	0.08347(6)	0.82276(12)	0.69617(19)	0.12758(8)	0.34539(16)	0.32638(19)	0.53257(16)	0.3327(27)	0.4483(11)	0.4467(21)	0.7119(34)	0.6559(29)	0.4898(37)	0.1346(28)
673	0.51971(15)	0.08345(6)	0.82262(12)	0.69608(19)	0.12761(8)	0.34570(16)	0.32619(19)	0.53243(16)	0.3325(27)	0.4482(11)	0.4465(21)	0.7125(35)	0.6557(29)	0.4896(37)	0.1350(28)
723	0.51972(14)	0.08345(6)	0.82259(12)	0.69605(19)	0.12762(8)	0.34575(16)	0.32614(18)	0.53240(15)	0.3324(27)	0.4482(11)	0.4465(20)	0.7125(34)	0.6558(29)	0.4897(36)	0.1350(28)
773	0.51970(14)	0.08336(6)	0.82233(12)	0.69606(19)	0.12760(8)	0.34606(16)	0.32575(18)	0.53186(15)	0.3320(26)	0.4483(11)	0.4464(20)	0.7122(34)	0.6559(29)	0.4891(36)	0.1354(28)
823	0.51970(14)	0.08336(6)	0.82233(12)	0.69606(19)	0.12760(8)	0.34606(16)	0.32575(18)	0.53186(15)	0.3320(26)	0.4483(11)	0.4464(20)	0.7122(33)	0.6559(28)	0.4891(35)	0.1354(27)
873	0.52003(14)	0.08330(6)	0.82193(12)	0.69597(19)	0.12747(8)	0.34655(16)	0.32513(18)	0.53153(15)	0.3319(25)	0.4484(10)	0.4465(19)	0.7120(32)	0.6559(27)	0.4891(34)	0.1354(26)
923	0.52019(14)	0.08325(6)	0.82174(12)	0.69580(19)	0.12753(8)	0.34674(16)	0.32505(18)	0.53145(15)	0.3319(24)	0.4484(10)	0.4465(19)	0.7121(31)	0.6558(27)	0.4890(34)	0.1355(26)
973	0.52019(14)	0.08325(6)	0.82174(12)	0.69580(18)	0.12753(8)	0.34674(16)	0.32504(18)	0.53145(15)	0.3319(25)	0.4484(10)	0.4465(19)	0.7121(31)	0.6558(26)	0.4891(33)	0.1355(26)
1023	0.52085(14)	0.08330(6)	0.82095(12)	0.69542(18)	0.12740(8)	0.34732(15)	0.32378(18)	0.53048(15)	0.3318(26)	0.4485(11)	0.4465(20)	0.7120(34)	0.6553(28)	0.4891(36)	0.1357(27)
1073	0.52103(14)	0.08327(6)	0.82070(12)	0.69537(19)	0.12754(8)	0.34770(15)	0.32308(19)	0.52993(15)	0.3319(27)	0.4486(11)	0.4464(21)	0.7117(35)	0.6551(29)	0.4890(38)	0.1357(29)
1123	0.52122(14)	0.08315(6)	0.82019(12)	0.69528(19)	0.12758(8)	0.34800(15)	0.32259(19)	0.52942(15)	0.3320(26)	0.4488(11)	0.4467(20)	0.7106(34)	0.6545(28)	0.4883(37)	0.1358(28)
1173	0.52152(15)	0.08306(6)	0.81952(12)	0.69506(19)	0.12767(8)	0.34853(15)	0.32209(20)	0.52908(16)	0.3318(28)	0.4489(12)	0.4471(23)	0.7109(39)	0.6540(31)	0.4878(41)	0.1358(31)

Table S6. Atomic coordinates of $Ca_3Eu_2(BO_3)_4$ structure versus temperature (part 2).

T [K]	O1x	O1y	O1z	O2x	O2y	O2z	O3x	O3y	O3z	O4x	O4y	O4z	O5x	O5y	O5z	O6x	O6z	O7x	O7z
295	0.5542(10)	0.1752(4)	0.0660(9)	0.7541(11)	0.3240(5)	0.7248(8)	0.4074(12)	0.4068(5)	0.5674(10)	0.2036(11)	0.5085(5)	0.4873(9)	0.3946(11)	0.4619(5)	0.3005(10)	0.3950(15)	0.2692(13)	0.6619(16)	0.5035(12)
323	0.5536(11)	0.1754(5)	0.0664(9)	0.7543(12)	0.3240(5)	0.7248(9)	0.4076(12)	0.4069(5)	0.5674(10)	0.2036(11)	0.5085(5)	0.4874(9)	0.3945(11)	0.4620(5)	0.3005(10)	0.3943(16)	0.2693(14)	0.6619(16)	0.5036(13)
373	0.5541(11)	0.1755(5)	0.0669(9)	0.7548(12)	0.3239(5)	0.7251(8)	0.4079(12)	0.4071(5)	0.5674(10)	0.2032(11)	0.5085(5)	0.4872(9)	0.3935(11)	0.4623(5)	0.3007(10)	0.3918(15)	0.2689(13)	0.6616(16)	0.5040(13)
423	0.5531(11)	0.1753(5)	0.0676(9)	0.7572(12)	0.3236(5)	0.7252(9)	0.4075(12)	0.4072(5)	0.5677(10)	0.2034(11)	0.5087(5)	0.4870(9)	0.3927(11)	0.4621(5)	0.3007(10)	0.3907(15)	0.2684(13)	0.6619(16)	0.5042(13)
473	0.5518(11)	0.1754(5)	0.0688(9)	0.7578(12)	0.3234(5)	0.7250(8)	0.4063(12)	0.4073(5)	0.5677(10)	0.2033(11)	0.5087(5)	0.4870(9)	0.3923(11)	0.4619(5)	0.3007(10)	0.3899(15)	0.2684(13)	0.6620(16)	0.5044(13)
523	0.5508(11)	0.1755(4)	0.0693(9)	0.7577(11)	0.3235(5)	0.7250(8)	0.4063(11)	0.4073(5)	0.5679(10)	0.2035(11)	0.5087(5)	0.4870(9)	0.3923(11)	0.4619(5)	0.3006(10)	0.3899(15)	0.2683(13)	0.6619(16)	0.5043(12)
573	0.5526(11)	0.1753(4)	0.0694(8)	0.7553(11)	0.3231(4)	0.7262(8)	0.4058(11)	0.4078(5)	0.5688(9)	0.2035(11)	0.5085(5)	0.4869(9)	0.3906(11)	0.4627(5)	0.3006(10)	0.3893(15)	0.2680(13)	0.6620(15)	0.5051(12)
623	0.5522(11)	0.1755(4)	0.0701(8)	0.7548(12)	0.3229(5)	0.7263(8)	0.4055(11)	0.4076(5)	0.5688(9)	0.2036(11)	0.5084(5)	0.4875(9)	0.3901(11)	0.4636(5)	0.3007(10)	0.3889(15)	0.2682(13)	0.6605(16)	0.5054(12)
673	0.5526(11)	0.1755(4)	0.0702(8)	0.7535(12)	0.3227(4)	0.7265(8)	0.4043(11)	0.4073(5)	0.5687(9)	0.2035(10)	0.5082(5)	0.4879(9)	0.3901(11)	0.4636(5)	0.3008(10)	0.3888(15)	0.2680(13)	0.6601(15)	0.5061(12)
723	0.5509(10)	0.1757(4)	0.0712(8)	0.7534(11)	0.3229(4)	0.7265(8)	0.4042(11)	0.4073(5)	0.5688(9)	0.2038(10)	0.5081(5)	0.4879(8)	0.3901(10)	0.4636(5)	0.3007(9)	0.3888(15)	0.2679(13)	0.6600(15)	0.5060(12)
773	0.5507(10)	0.1751(4)	0.0701(8)	0.7522(11)	0.3235(4)	0.7261(8)	0.4045(11)	0.4073(5)	0.5693(9)	0.2046(10)	0.5080(5)	0.4879(8)	0.3899(10)	0.4628(5)	0.3005(9)	0.3880(14)	0.2676(13)	0.6585(15)	0.5061(12)
823	0.5507(10)	0.1751(4)	0.0701(8)	0.7522(11)	0.3235(4)	0.7261(8)	0.4045(11)	0.4073(5)	0.5693(9)	0.2046(10)	0.5080(5)	0.4879(8)	0.3899(10)	0.4628(5)	0.3005(9)	0.3880(14)	0.2676(12)	0.6585(15)	0.5061(12)
873	0.5500(10)	0.1754(4)	0.0690(8)	0.7511(11)	0.3234(4)	0.7259(8)	0.4041(11)	0.4071(5)	0.5692(9)	0.2054(10)	0.5080(5)	0.4881(8)	0.3898(10)	0.4625(5)	0.3005(9)	0.3871(14)	0.2675(12)	0.6562(14)	0.5062(12)
923	0.5496(10)	0.1753(4)	0.0698(8)	0.7512(11)	0.3234(4)	0.7258(8)	0.4034(11)	0.4072(4)	0.5693(9)	0.2059(10)	0.5080(5)	0.4882(8)	0.3901(10)	0.4627(5)	0.3005(9)	0.3867(14)	0.2674(12)	0.6546(14)	0.5063(11)
973	0.5494(10)	0.1753(4)	0.0698(8)	0.7512(12)	0.3235(4)	0.7258(7)	0.4034(11)	0.4072(5)	0.5693(9)	0.2059(10)	0.5080(5)	0.4882(8)	0.3901(11)	0.4627(4)	0.3005(9)	0.3867(14)	0.2674(12)	0.6546(15)	0.5063(11)
1023	0.5481(10)	0.1759(4)	0.0723(8)	0.7517(11)	0.3242(4)	0.7257(8)	0.4011(11)	0.4073(5)	0.5697(9)	0.2063(10)	0.5081(5)	0.4876(8)	0.3901(10)	0.4622(5)	0.3002(9)	0.3863(14)	0.2666(12)	0.6525(14)	0.5069(12)
1073	0.5474(10)	0.1760(4)	0.0719(8)	0.7501(11)	0.3243(4)	0.7252(8)	0.3995(11)	0.4072(5)	0.5700(9)	0.2069(10)	0.5084(5)	0.4868(9)	0.3898(10)	0.4619(5)	0.3001(9)	0.3852(14)	0.2663(12)	0.6514(14)	0.5070(12)
1123	0.5461(10)	0.1763(4)	0.0703(8)	0.7509(11)	0.3242(4)	0.7234(8)	0.4000(11)	0.4074(5)	0.5698(9)	0.2080(10)	0.5091(5)	0.4860(9)	0.3872(10)	0.4607(5)	0.2995(9)	0.3823(14)	0.2651(13)	0.6496(14)	0.5070(12)
1173	0.5461(11)	0.1764(4)	0.0701(8)	0.7492(12)	0.3241(4)	0.7230(8)	0.4023(11)	0.4075(5)	0.5690(9)	0.2082(10)	0.5091(5)	0.4859(9)	0.3864(10)	0.4599(5)	0.2997(9)	0.3817(14)	0.2650(13)	0.6466(14)	0.5076(12)

Figure S1 DTA-TGA measurement of $Ca_3Eu_2(BO_3)_4$, heating ramp.