Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2017

$M_3V_2B_{10}O_{23}$ (M = Ca, Sr): Two new vanadoborates with new $[V_2B_{10}O_{23}]_\infty$ double layers

Zhaohui Chen[a*], Yaqin Liu[a], Yunjing Shi[b], Wenyao Zhang[a], Qun Jing[a,c], Yuan Fang[a], Xiaoyu Dong[b*]

[a]Physical and Chemical Detecting Center, Xinjiang University, 666 Shengli Road, Urumqi 830046, China;

[b]Engineering Department of Chemistry and Environment, Xinjiang Institute of Engineering, 236 Nanchang Road, Urumqi 830091, China

[c]Department of Physics, College of Sciences, Shihezi University, Shihezi, 832000, China;

*To whom correspondence should be addressed. Phone: (86)991-8582966. Fax: (86)991-8582966. E-mail: chenzhaohui686@sina.cn (Z. Chen).

Table S1 Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $Ca_3V_2B_{10}O_{23}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x/a	y/b	z/c	U(eq)	Occ.	BVS
Ca(1)	1932(2)	7454(1)	-14(1)	6(1)	1	1.960
Ca(2)	4499(2)	6226(1)	4028(1)	12(1)	1	1.881
Ca(3)	466(2)	8780(1)	6016(1)	12(1)	1	1.908
V(1)	3586(2)	4630(1)	686(1)	22(1)	1	5.237
V(2)	-3150(2)	9381(2)	655(1)	55(1)	1	5.023
B(1)	1981(10)	8784(6)	3213(6)	11(1)	1	3.084
B(2)	9164(10)	7603(6)	3460(6)	10(1)	1	3.108
B(3)	2711(10)	5989(6)	6339(6)	11(1)	1	3.064
B(4)	-705(10)	6612(6)	6753(6)	11(1)	1	3.052
B(5)	-4122(10)	7465(6)	6621(6)	9(1)	1	3.091
B(6)	-4730(10)	9437(6)	6307(6)	10(1)	1	3.034
B(7)	502(11)	2924(7)	-1476(6)	19(2)	1	3.054
B(8)	-161(10)	5636(6)	3818(6)	11(1)	1	3.027
B(9)	4177(10)	11407(6)	6269(6)	11(1)	1	3.054
B(10)	-1849(11)	7975(6)	-1446(6)	15(1)	1	3.058
O(1)	-1279(7)	8616(4)	-225(4)	23(1)	1	2.140
O(2)	-3672(7)	8120(4)	-2110(4)	17(1)	1	1.943
O(3)	1141(7)	8049(4)	1906(4)	17(1)	1	2.019
O(4)	1077(8)	3625(5)	-258(4)	27(1)	1	2.176
O(5)	7309(6)	7842(4)	3963(4)	14(1)	1	2.076
O(6)	3809(6)	8184(4)	3620(4)	14(1)	1	2.040
O(7)	371(6)	8823(4)	3820(3)	11(1)	1	1.905
O(8)	3674(6)	10231(4)	6271(4)	13(1)	1	2.158
O(9)	-2679(6)	9869(4)	6525(4)	14(1)	1	2.140
O(10)	-2221(6)	7220(4)	6190(3)	10(1)	1	1.908
O(11)	1315(6)	6847(4)	6511(4)	14(1)	1	2.067
O(12)	4617(6)	6166(4)	6128(4)	13(1)	1	1.994
O(13)	1318(6)	4804(4)	3716(4)	13(1)	1	2.017
O(14)	490(6)	6877(4)	4074(4)	14(1)	1	2.050
O(15)	7761(6)	5230(4)	3719(4)	14(1)	1	2.150
O(16)	-427(7)	7176(4)	-1934(4)	14(1)	1	1.975
O(17)	-5446(6)	8209(4)	6057(4)	12(1)	1	2.043
O(18)	1451(7)	3193(4)	-2195(4)	21(1)	1	1.909
O(19)	-3899(15)	8204(9)	1261(8)	25(2)	0.5	0.432
O(20)	-1849(9)	10387(5)	1922(5)	38(1)	1	2.265
O(21)	-5985(14)	9273(9)	-30(8)	21(2)	0.5	0.857
O(22)	4106(15)	5718(8)	34(8)	22(2)	0.5	0.981

O(23)	3158(16)	5547(8)	2001(8)	24(2)	0.5	0.931
O(24)	-5093(16)	8619(11)	474(11)	36(3)	0.5	1.604
O(25)	5438(19)	3832(11)	970(10)	45(3)	0.5	0.901
O(26)	4100(20)	4629(14)	1945(10)	48(3)	0.5	1.096
O(27)	3110(20)	6060(13)	860(13)	56(4)	0.5	1.165

Table S2 Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $Sr_3V_2B_{10}O_{23}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x/a	y/b	z/c	U(eq)	Occ.	BVS
Sr(1)	1942(1)	7474(1)	-45(1)	13(1)	1	2.162
Sr(2)	4544(1)	6176(1)	4010(1)	12(1)	1	2.227
Sr(3)	484(1)	8840(1)	6034(1)	12(1)	1	2.160
V(1)	3502(2)	4565(1)	611(1)	20(1)	1	5.306
V(2)	2990(2)	10487(2)	-592(1)	26(1)	1	5.230
B(1)	2027(12)	8742(7)	3213(7)	11(2)	1	3.083
B(2)	9184(11)	7576(7)	3444(7)	8(1)	1	3.095
B(3)	2641(12)	6063(8)	6383(7)	10(2)	1	3.045
B(4)	-835(11)	6597(7)	6708(6)	8(1)	1	3.030
B(5)	-4202(12)	7495(7)	6611(7)	10(2)	1	3.075
B(6)	-4731(12)	9482(7)	6324(7)	11(2)	1	3.025
B(7)	436(13)	2905(8)	-1526(8)	18(2)	1	3.085
B(8)	-154(12)	5593(8)	3805(7)	11(2)	1	3.071
B(9)	4173(12)	11434(8)	6278(7)	11(2)	1	3.100
B(10)	-1934(13)	7943(8)	-1509(7)	16(2)	1	3.037
O(1)	1367(9)	11447(6)	313(5)	32(2)	1	2.263
O(2)	-3676(7)	8173(5)	-2134(4)	14(1)	1	1.892
O(3)	1192(8)	8021(5)	1945(4)	16(1)	1	2.099
O(4)	1066(9)	3589(6)	-328(5)	31(2)	1	2.224
O(5)	7334(7)	7837(4)	3940(4)	10(1)	1	2.092
O(6)	3858(7)	8151(5)	3599(5)	14(1)	1	2.109
O(7)	462(7)	8772(4)	3826(4)	9(1)	1	1.949
O(8)	3709(7)	10273(5)	6267(5)	14(1)	1	2.224
O(9)	-2711(7)	9928(4)	6525(4)	11(1)	1	2.097
O(10)	-2360(7)	7193(4)	6164(4)	8(1)	1	1.941
O(11)	1179(7)	6887(5)	6507(5)	13(1)	1	2.064
O(12)	4494(7)	6247(4)	6184(4)	11(1)	1	2.093
O(13)	1358(7)	4812(4)	3799(5)	13(1)	1	2.111
O(14)	416(7)	6805(4)	4005(4)	11(1)	1	2.094
O(15)	7816(7)	5136(4)	3651(4)	12(1)	1	2.221
O(16)	-598(8)	7110(5)	-2014(4)	17(1)	1	1.993
O(17)	-5431(7)	8281(4)	6098(4)	10(1)	1	2.121
O(18)	1449(8)	3149(5)	-2213(4)	17(1)	1	1.946
O(19)	1450(20)	9601(10	-1839(9)	23(3)	0.5	1.060
O(20)	5874(16)	10697(10)	50(9)	16(2)	0.5	0.978
O(21)	4207(16)	5706(10)	93(10)	18(2)	0.5	0.998
O(22)	3046(19)	5450(11)	1904(9)	27(3)	0.5	0.920

O(23)	4570(20)	11355(13)	-718(13)	37(3)	0.5	1.264
O(24)	5160(20)	3689(12)	820(13)	36(3)	0.5	1.147
O(25)	4200(20)	4410(13)	1823(12)	38(3)	0.5	0.928
O(26)	3050(20)	5966(15)	891(14)	48(4)	0.5	1.137
O(27)	2720(50)	10750(40)	-1710(20)	19(20)	0.5	0.985
O(28)	2170(30)	9070(18)	-900(20)	93(8)	0.5	1.073

Table S3 Selected bond lengths [Å] and angles [deg.] for $Ca_3V_2B_{10}O_{23}$.

Ca(1)-O(24)#1	2.153(10)	O(6)-Ca(2)-O(5)	52.70(13)
Ca(1)-O(27)	2.335(13)	O(23)-Ca(2)-O(17)#1	140.0(3)
Ca(1)-O(3)	2.434(4)	O(15)-Ca(2)-O(17)#1	120.51(14)
Ca(1)-O(16)	2.451(4)	O(26)-Ca(2)-O(17)#1	168.9(3)
Ca(1)-O(22)	2.468(9)	O(13)-Ca(2)-O(17)#1	102.33(13)
Ca(1)-O(4)#2	2.474(5)	O(6)-Ca(2)-O(17)#1	71.18(13)
Ca(1)-O(26)#3	2.484(12)	O(5)-Ca(2)-O(17)#1	81.51(13)
Ca(1)-O(21)#1	2.488(9)	O(23)-Ca(2)-O(12)	153.4(3)
Ca(1)-O(1)	2.514(5)	O(15)-Ca(2)-O(12)	97.86(13)
Ca(1)-O(19)#1	2.738(10)	O(26)-Ca(2)-O(12)	136.6(3)
Ca(2)-O(23)	2.301(9)	O(13)-Ca(2)-O(12)	72.70(13)
Ca(2)-O(15)	2.462(4)	O(6)-Ca(2)-O(12)	123.60(13)
Ca(2)-O(27)	2.476(12)	O(5)-Ca(2)-O(12)	118.66(13)
Ca(2)-O(13)	2.476(4)	O(17)#1-Ca(2)-O(12)	53.10(12)
Ca(2)-O(6)	2.524(4)	O(23)-Ca(2)-O(14)	83.0(3)
Ca(2)-O(5)	2.632(4)	O(15)-Ca(2)-O(14)	169.12(14)
Ca(2)-O(17)#1	2.643(4)	O(26)-Ca(2)-O(14)	104.2(3)
Ca(2)-O(12)	2.682(4)	O(13)-Ca(2)-O(14)	52.68(12)
Ca(2)-O(14)	2.735(4)	O(6)-Ca(2)-O(14)	67.18(13)
Ca(2)-O(12)#4	2.743(4)	O(5)-Ca(2)-O(14)	118.90(13)
Ca(2)-O(10)#1	2.836(4)	O(17)#1-Ca(2)-O(14)	69.21(12)
Ca(3)-O(20)#5	2.327(5)	O(12)-Ca(2)-O(14)	84.23(13)
Ca(3)-O(9)	2.491(4)	O(23)-Ca(2)-O(12)#4	94.7(2)
Ca(3)-O(8)	2.535(4)	O(15)-Ca(2)-O(12)#4	52.42(12)
Ca(3)-O(14)	2.544(4)	O(26)-Ca(2)-O(12)#4	67.2(3)
Ca(3)-O(11)	2.572(4)	O(13)-Ca(2)-O(12)#4	66.79(13)
Ca(3)-O(10)	2.600(4)	O(6)-Ca(2)-O(12)#4	164.84(14)
Ca(3)-O(5)#6	2.708(4)	O(5)-Ca(2)-O(12)#4	121.83(13)
Ca(3)-O(7)#5	2.740(4)	O(17)#1-Ca(2)-O(12)#4	123.58(13)
Ca(3)-O(17)#1	2.747(4)	O(12)-Ca(2)-O(12)#4	71.53(14)
Ca(3)-O(7)	2.799(4)	O(14)-Ca(2)-O(12)#4	119.09(12)
V(1)-O(26)	1.557(11)	O(23)-Ca(2)-O(10)#1	154.1(3)
V(1)-O(25)	1.585(12)	O(15)-Ca(2)-O(10)#1	69.40(13)
V(1)-O(27)	1.605(13)	O(26)-Ca(2)-O(10)#1	136.4(3)
V(1)-O(23)	1.664(9)	O(13)-Ca(2)-O(10)#1	122.42(13)
V(1)-O(22)	1.824(9)	O(6)-Ca(2)-O(10)#1	102.92(13)
V(1)-O(4)	1.830(5)	O(5)-Ca(2)-O(10)#1	69.99(12)
V(1)-O(22)#3	1.905(9)	O(17)#1-Ca(2)-O(10)#1	51.90(12)
V(2)-O(24)	1.449(10)	O(12)-Ca(2)-O(10)#1	50.28(12)
V(2)-O(20)	1.568(5)	O(14)-Ca(2)-O(10)#1	119.07(12)
V(2)-O(21)	1.828(9)	O(12)#4-Ca(2)-O(10)#1	86.20(12)
V(2)-O(1)	1.838(5)	O(20)#5-Ca(3)-O(9)	84.21(18)

V(2)-O(19)	1.915(10)	O(20)#5-Ca(3)-O(8)	80.08(17)
V(2)-O(21)#7	2.034(10)	O(9)-Ca(3)-O(8)	116.00(14)
B(1)-O(7)	1.434(8)	O(20)#5-Ca(3)-O(14)	142.59(18)
B(1)-O(6)	1.477(8)	O(9)-Ca(3)-O(14)	126.41(14)
B(1)-O(3)	1.479(8)	O(8)-Ca(3)-O(14)	100.37(14)
B(1)-O(9)#5	1.481(7)	O(20)#5-Ca(3)-O(11)	73.49(18)
B(2)-O(18)#3	1.437(8)	O(9)-Ca(3)-O(11)	118.61(14)
B(2)-O(7)#1	1.439(7)	O(8)-Ca(3)-O(11)	115.17(13)
B(2)-O(5)	1.476(7)	O(14)-Ca(3)-O(11)	72.68(13)
B(2)-O(14)#1	1.510(7)	O(20)#5-Ca(3)-O(10)	88.19(17)
B(3)-O(11)	1.334(8)	O(9)-Ca(3)-O(10)	69.90(13)
B(3)-O(12)	1.362(8)	O(8)-Ca(3)-O(10)	165.99(14)
B(3)-O(15)#4	1.396(8)	O(14)-Ca(3)-O(10)	84.30(13)
B(4)-O(10)	1.437(8)	O(11)-Ca(3)-O(10)	53.36(12)
B(4)-O(11)	1.469(7)	O(20)#5-Ca(3)-O(5)#6	154.66(17)
B(4)-O(16)#8	1.487(7)	O(9)-Ca(3)-O(5)#6	73.94(13)
B(4)-O(13)#9	1.494(7)	O(8)-Ca(3)-O(5)#6	120.87(13)
B(5)-O(2)#8	1.426(8)	O(14)-Ca(3)-O(5)#6	53.40(13)
B(5)-O(10)	1.456(7)	O(11)-Ca(3)-O(5)#6	105.69(13)
B(5)-O(17)	1.486(7)	O(10)-Ca(3)-O(5)#6	72.52(12)
B(5)-O(12)#6	1.502(7)	O(20)#5-Ca(3)-O(7)#5	90.67(17)
B(6)-O(9)	1.346(8)	O(9)-Ca(3)-O(7)#5	53.05(12)
B(6)-O(17)	1.361(8)	O(8)-Ca(3)-O(7)#5	65.51(12)
B(6)-O(8)#6	1.395(8)	O(14)-Ca(3)-O(7)#5	123.93(13)
B(7)-O(18)	1.345(9)	O(11)-Ca(3)-O(7)#5	163.38(13)
B(7)-O(4)	1.374(8)	O(10)-Ca(3)-O(7)#5	122.72(13)
B(7)-O(3)#2	1.375(8)	O(5)#6-Ca(3)-O(7)#5	86.39(12)
B(8)-O(13)	1.354(8)	O(20)#5-Ca(3)-O(17)#1	81.74(17)
B(8)-O(14)	1.361(8)	O(9)-Ca(3)-O(17)#1	162.90(14)
B(8)-O(15)#6	1.389(8)	O(8)-Ca(3)-O(17)#1	51.83(12)
B(9)-O(6)#10	1.347(8)	O(14)-Ca(3)-O(17)#1	70.41(13)
B(9)-O(5)#10	1.363(8)	O(11)-Ca(3)-O(17)#1	66.30(13)
B(9)-O(8)	1.384(8)	O(10)-Ca(3)-O(17)#1	119.15(13)
B(10)-O(2)	1.342(8)	O(5)#6-Ca(3)-O(17)#1	121.78(13)
B(10)-O(1)	1.370(8)	O(7)#5-Ca(3)-O(17)#1	117.28(12)
B(10)-O(16)	1.381(8)	O(20)#5-Ca(3)-O(7)	150.29(17)
O(2)-B(5)#11	1.426(8)	O(9)-Ca(3)-O(7)	102.80(13)
O(3)-B(7)#2	1.375(8)	O(8)-Ca(3)-O(7)	70.85(13)
O(4)-Ca(1)#2	2.474(5)	O(14)-Ca(3)-O(7)	52.67(12)
O(5)-B(9)#10	1.363(8)	O(7)-B(1)-O(3)	111.3(5)
O(5)-Ca(3)#1	2.708(4)	O(6)-B(1)-O(3)	108.2(5)
O(6)-B(9)#10	1.347(8)	O(11)-Ca(3)-O(7)	124.43(13)
O(7)-B(2)#6	1.439(7)	O(10)-Ca(3)-O(7)	121.43(12)
O(7)-Ca(3)#5	2.740(4)	O(5)#6-Ca(3)-O(7)	50.78(12)

O(8)-B(6)#1	1.395(8)	O(7)#5-Ca(3)-O(7)	72.04(13)
O(9)-B(1)#5	1.481(7)	O(17)#1-Ca(3)-O(7)	85.02(12)
O(10)-Ca(2)#6	2.836(4)	O(26)-V(1)-O(25)	63.6(7)
O(12)-B(5)#1	1.502(7)	O(26)-V(1)-O(27)	107.0(7)
O(12)-Ca(2)#4	2.743(4)	O(25)-V(1)-O(27)	142.2(7)
O(13)-B(4)#9	1.494(7)	O(26)-V(1)-O(23)	43.9(6)
O(14)-B(2)#6	1.510(7)	O(25)-V(1)-O(23)	105.2(5)
O(15)-B(8)#1	1.389(8)	O(27)-V(1)-O(23)	65.5(6)
O(15)-B(3)#4	1.396(8)	O(26)-V(1)-O(22)	137.7(6)
O(16)-B(4)#11	1.487(7)	O(25)-V(1)-O(22)	117.4(6)
O(17)-Ca(2)#6	2.643(4)	O(27)-V(1)-O(22)	43.6(5)
O(17)-Ca(3)#6	2.747(4)	O(23)-V(1)-O(22)	106.3(4)
O(18)-B(2)#3	1.437(8)	O(26)-V(1)-O(4)	110.4(5)
O(19)-O(24)	1.364(14)	O(25)-V(1)-O(4)	113.5(4)
O(19)-Ca(1)#6	2.738(10)	O(27)-V(1)-O(4)	104.2(6)
O(20)-Ca(3)#5	2.327(5)	O(23)-V(1)-O(4)	106.7(4)
O(21)-V(2)#7	2.034(10)	O(22)-V(1)-O(4)	107.0(3)
O(21)-Ca(1)#6	2.488(9)	O(26)-V(1)-O(22)#3	113.8(6)
O(22)-V(1)#3	1.905(9)	O(25)-V(1)-O(22)#3	55.2(5)
O(24)-Ca(1)#6	2.153(10)	O(27)-V(1)-O(22)#3	106.0(5)
O(26)-Ca(1)#3	2.484(12)	O(23)-V(1)-O(22)#3	138.6(4)
O(24)#1-Ca(1)-O(27)	98.5(5)	O(22)-V(1)-O(22)#3	65.3(5)
O(24)#1-Ca(1)-O(3)	102.5(3)	O(4)-V(1)-O(22)#3	114.6(3)
O(27)-Ca(1)-O(3)	67.4(3)	O(24)-V(2)-O(20)	122.5(5)
O(24)#1-Ca(1)-O(16)	113.9(3)	O(24)-V(2)-O(21)	42.6(5)
O(27)-Ca(1)-O(16)	134.5(4)	O(20)-V(2)-O(21)	127.0(4)
O(3)-Ca(1)-O(16)	129.33(15)	O(24)-V(2)-O(1)	118.6(5)
O(24)#1-Ca(1)-O(22)	85.8(4)	O(20)-V(2)-O(1)	108.6(3)
O(27)-Ca(1)-O(22)	31.0(4)	O(21)-V(2)-O(1)	122.3(3)
O(3)-Ca(1)-O(22)	97.7(2)	O(24)-V(2)-O(19)	45.3(5)
O(16)-Ca(1)-O(22)	118.3(2)	O(20)-V(2)-O(19)	93.0(4)
O(24)#1-Ca(1)-O(4)#2	158.1(3)	O(21)-V(2)-O(19)	87.3(4)
O(27)-Ca(1)-O(4)#2	69.1(4)	O(1)-V(2)-O(19)	105.7(3)
O(3)-Ca(1)-O(4)#2	56.46(14)	O(24)-V(2)-O(21)#7	106.6(5)
O(16)-Ca(1)-O(4)#2	86.68(15)	O(20)-V(2)-O(21)#7	94.6(3)
O(22)-Ca(1)-O(4)#2	91.0(3)	O(21)-V(2)-O(21)#7	64.2(5)
O(24)#1-Ca(1)-O(25)#3	68.5(4)	O(1)-V(2)-O(21)#7	100.4(3)
O(27)-Ca(1)-O(25)#3	69.7(4)	O(19)-V(2)-O(21)#7	148.8(4)
O(3)-Ca(1)-O(25)#3	134.1(3)	O(7)-B(1)-O(6)	111.4(5)
O(16)-Ca(1)-O(25)#3	92.9(3)	O(7)-B(1)-O(3)	111.3(5)
O(22)-Ca(1)-O(25)#3	38.7(4)	O(6)-B(1)-O(3)	108.2(5)
O(4)#2-Ca(1)-O(25)#3	120.1(3)	O(7)-B(1)-O(9)#5	107.2(5)
O(24)#1-Ca(1)-O(21)#1	29.9(3)	O(6)-B(1)-O(9)#5	109.9(5)
O(27)-Ca(1)-O(21)#1	128.5(4)	O(3)-B(1)-O(9)#5	108.8(5)

O(3)-Ca(1)-O(21)#1	111.2(2)	O(18)#3-B(2)-O(7)#1	115.3(5)
O(16)-Ca(1)-O(21)#1	88.2(2)	O(18)#3-B(2)-O(5)	111.7(5)
O(22)-Ca(1)-O(21)#1	112.0(3)	O(7)#1-B(2)-O(5)	108.3(5)
O(4)#2-Ca(1)-O(21)#1	156.0(2)	O(18)#3-B(2)-O(14)#1	108.6(5)
O(25)#3-Ca(1)-O(21)#1	83.6(4)	O(7)#1-B(2)-O(14)#1	107.7(5)
O(24)#1-Ca(1)-O(1)	114.1(3)	O(5)-B(2)-O(14)#1	104.7(4)
O(27)-Ca(1)-O(1)	136.7(3)	O(11)-B(3)-O(12)	124.7(5)
O(3)-Ca(1)-O(1)	77.96(15)	O(11)-B(3)-O(15)#4	121.2(5)
O(16)-Ca(1)-O(1)	55.84(14)	O(12)-B(3)-O(15)#4	113.9(5)
O(22)-Ca(1)-O(1)	160.1(2)	O(10)-B(4)-O(11)	106.1(5)
O(4)#2-Ca(1)-O(1)	70.31(17)	O(10)-B(4)-O(16)#8	111.5(5)
O(25)#3-Ca(1)-O(1)	147.7(3)	O(11)-B(4)-O(16)#8	109.2(5)
O(21)#1-Ca(1)-O(1)	87.4(2)	O(10)-B(4)-O(13)#9	112.9(5)
O(24)#1-Ca(1)-O(19)#1	29.4(3)	O(11)-B(4)-O(13)#9	109.7(5)
O(27)-Ca(1)-O(19)#1	69.7(4)	O(16)#8-B(4)-O(13)#9	107.4(5)
O(3)-Ca(1)-O(19)#1	86.2(2)	O(2)#8-B(5)-O(10)	113.3(5)
O(16)-Ca(1)-O(19)#1	140.3(2)	O(2)#8-B(5)-O(17)	110.1(5)
O(22)-Ca(1)-O(19)#1	63.6(3)	O(10)-B(5)-O(17)	109.6(5)
O(4)#2-Ca(1)-O(19)#1	132.4(2)	O(2)#8-B(5)-O(12)#6	112.7(5)
O(25)#3-Ca(1)-O(19)#1	64.0(3)	O(10)-B(5)-O(12)#6	105.1(4)
O(21)#1-Ca(1)-O(19)#1	59.0(3)	O(17)-B(5)-O(12)#6	105.6(4)
O(1)-Ca(1)-O(19)#1	134.5(2)	O(9)-B(6)-O(17)	124.4(5)
O(23)-Ca(2)-O(15)	90.7(3)	O(9)-B(6)-O(8)#6	121.2(5)
O(23)-Ca(2)-O(26)	29.0(4)	O(17)-B(6)-O(8)#6	114.4(5)
O(15)-Ca(2)-O(26)	67.0(3)	O(18)-B(7)-O(4)	122.1(6)
O(23)-Ca(2)-O(13)	81.1(3)	O(18)-B(7)-O(3)#2	122.6(6)
O(15)-Ca(2)-O(13)	117.67(14)	O(4)-B(7)-O(3)#2	115.3(6)
O(26)-Ca(2)-O(13)	79.2(3)	O(13)-B(8)-O(14)	117.7(5)
O(23)-Ca(2)-O(6)	71.7(2)	O(13)-B(8)-O(15)#6	120.1(5)
O(15)-Ca(2)-O(6)	119.21(14)	O(14)-B(8)-O(15)#6	122.1(5)
O(26)-Ca(2)-O(6)	98.2(3)	O(6)#10-B(9)-O(5)#10	115.4(5)
O(13)-Ca(2)-O(6)	116.13(14)	O(6)#10-B(9)-O(8)	120.8(5)
O(23)-Ca(2)-O(5)	87.9(3)	O(5)#10-B(9)-O(8)	123.4(5)
O(15)-Ca(2)-O(5)	69.48(13)	O(2)-B(10)-O(1)	121.6(6)
O(26)-Ca(2)-O(5)	94.6(3)	O(2)-B(10)-O(16)	122.9(6)
O(13)-Ca(2)-O(5)	166.73(14)	O(1)-B(10)-O(16)	115.4(6)

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 -x,-y+1,-z #3 -x+1,-y+1,-z #4 -x+1,-y+1,-z+1 #5 -x,-y+2,-z+1 #6 x-1,y,z #7 -x-1,-y+2,-z #8 x,y,z+1 #9 -x,-y+1,-z+1 #10 -x+1,-y+2,-z+1 #11 x,y,z-1

Table S4 Selected bond lengths [Å] and angles [deg.] for $Sr_3V_2B_{10}O_{23}$.

Sr(1)-O(23)#1	2.445(14)	O(5)-Sr(2)-O(17)#5	80.78(14)
Sr(1)-O(24)#2	2.519(13)	O(22)-Sr(2)-O(12)	152.0(3)
Sr(1)-O(26)	2.534(16)	O(13)-Sr(2)-O(12)	70.24(15)
Sr(1)-O(28)	2.540(3)	O(15)-Sr(2)-O(12)	102.12(15)
Sr(1)-O(20)#1	2.559(10)	O(6)-Sr(2)-O(12)	120.48(15)
Sr(1)-O(1)#3	2.560(6)	O(25)-Sr(2)-O(12)	138.0(3)
Sr(1)-O(3)	2.568(5)	O(5)-Sr(2)-O(12)	118.44(14)
Sr(1)-O(4)#4	2.576(5)	O(17)#5-Sr(2)-O(12)	50.81(14)
Sr(1)-O(16)	2.585(5)	O(22)-Sr(2)-O(12)#6	94.2(3)
Sr(1)-O(21)	2.589(11)	O(13)-Sr(2)-O(12)#6	68.91(14)
Sr(2)-O(22)	2.454(11)	O(15)-Sr(2)-O(12)#6	51.08(14)
Sr(2)-O(13)	2.523(5)	O(6)-Sr(2)-O(12)#6	163.41(16)
Sr(2)-O(15)	2.536(5)	O(25)-Sr(2)-O(12)#6	64.7(3)
Sr(2)-O(6)	2.572(5)	O(5)-Sr(2)-O(12)#6	121.33(14)
Sr(2)-O(25)	2.686(14)	O(17)#5-Sr(2)-O(12)#6	125.23(14)
Sr(2)-O(5)	2.702(5)	O(12)-Sr(2)-O(12)#6	76.06(15)
Sr(2)-O(17)#5	2.798(5)	O(22)-Sr(2)-O(10)#5	157.7(3)
Sr(2)-O(12)	2.802(5)	O(13)-Sr(2)-O(10)#5	119.09(15)
Sr(2)-O(12)#6	2.802(5)	O(15)-Sr(2)-O(10)#5	72.40(15)
Sr(2)-O(10)#5	2.836(5)	O(6)-Sr(2)-O(10)#5	102.70(15)
Sr(2)-O(14)	2.839(5)	O(25)-Sr(2)-O(10)#5	137.0(3)
Sr(3)-O(19)#7	2.449(11)	O(5)-Sr(2)-O(10)#5	71.44(14)
Sr(3)-O(9)	2.548(5)	O(17)#5-Sr(2)-O(10)#5	50.58(13)
Sr(3)-O(8)	2.581(5)	O(12)-Sr(2)-O(10)#5	49.51(13)
Sr(3)-O(11)	2.594(5)	O(12)#6-Sr(2)-O(10)#5	87.04(14)
Sr(3)-O(14)	2.707(5)	O(22)-Sr(2)-O(14)	80.0(3)
Sr(3)-O(10)	2.754(5)	O(13)-Sr(2)-O(14)	50.77(15)
Sr(3)-O(7)#8	2.780(5)	O(15)-Sr(2)-O(14)	167.02(15)
Sr(3)-O(17)#5	2.783(5)	O(6)-Sr(2)-O(14)	67.56(14)
Sr(3)-O(5)#9	2.804(5)	O(25)-Sr(2)-O(14)	103.8(3)
Sr(3)-O(7)	2.835(5)	O(5)-Sr(2)-O(14)	118.58(14)
Sr(3)-O(27)#7	2.88(4)	O(17)#5-Sr(2)-O(14)	70.40(14)
V(1)-O(24)	1.555(13)	O(12)-Sr(2)-O(14)	82.25(14)
V(1)-O(26)	1.556(15)	O(12)#6-Sr(2)-O(14)	119.66(13)
V(1)-O(25)	1.620(14)	O(10)#5-Sr(2)-O(14)	118.52(13)
V(1)-O(22)	1.669(12)	O(19)#7-Sr(3)-O(9)	79.7(3)
V(1)-O(21)	1.812(10)	O(19)#7-Sr(3)-O(8)	87.9(3)
V(1)-O(4)	1.819(6)	O(9)-Sr(3)-O(8)	117.26(15)
V(1)-O(21)#2	1.914(10)	O(19)#7-Sr(3)-O(11)	71.8(3)
V(2)-O(23)	1.526(14)	O(9)-Sr(3)-O(11)	116.65(15)
V(2)-O(28)	1.58(2)	O(8)-Sr(3)-O(11)	116.79(15)
V(2)-O(27)	1.577(17)	O(19)#7-Sr(3)-O(14)	143.4(3)

V(2)-O(19)	1.606(11)	O(9)-Sr(3)-O(14)	124.29(15)
V(2)-O(1)	1.818(6)	O(8)-Sr(3)-O(14)	101.24(16)
V(2)-O(20)	1.873(10)	O(11)-Sr(3)-O(14)	72.48(16)
V(2)-O(20)#1	1.874(11)	O(19)#7-Sr(3)-O(10)	82.4(3)
B(1)-O(7)	1.440(9)	O(9)-Sr(3)-O(10)	69.36(14)
B(1)-O(3)	1.469(9)	O(8)-Sr(3)-O(10)	167.07(16)
B(1)-O(9)#8	1.474(8)	O(11)-Sr(3)-O(10)	51.94(14)
B(1)-O(6)	1.488(9)	O(14)-Sr(3)-O(10)	82.00(14)
B(2)-O(18)#2	1.421(9)	O(19)#7-Sr(3)-O(7)#8	92.7(3)
B(2)-O(7)#5	1.450(8)	O(9)-Sr(3)-O(7)#8	52.22(14)
B(2)-O(5)	1.492(8)	O(8)-Sr(3)-O(7)#8	67.54(14)
B(2)-O(14)#5	1.507(9)	O(11)-Sr(3)-O(7)#8	163.22(15)
B(3)-O(12)	1.347(8)	O(14)-Sr(3)-O(7)#8	123.64(14)
B(3)-O(11)	1.354(9)	O(10)-Sr(3)-O(7)#8	121.18(13)
B(3)-O(15)#6	1.398(9)	O(19)#7-Sr(3)-O(17)#5	87.1(3)
B(4)-O(10)	1.443(9)	O(9)-Sr(3)-O(17)#5	162.95(15)
B(4)-O(11)	1.482(8)	O(8)-Sr(3)-O(17)#5	50.92(14)
B(4)-O(16)#7	1.484(9)	O(11)-Sr(3)-O(17)#5	68.36(14)
B(4)-O(13)#11	1.488(9)	O(14)-Sr(3)-O(17)#5	72.56(14)
B(5)-O(2)#7	1.441(9)	O(10)-Sr(3)-O(17)#5	119.74(14)
B(5)-O(10)	1.456(9)	O(7)#8-Sr(3)-O(17)#5	118.44(13)
B(5)-O(17)	1.482(9)	O(19)#7-Sr(3)-O(5)#9	147.9(3)
B(5)-O(12)#9	1.497(9)	O(9)-Sr(3)-O(5)#9	74.30(15)
B(6)-O(17)	1.351(9)	O(8)-Sr(3)-O(5)#9	120.64(16)
B(6)-O(9)	1.361(9)	O(11)-Sr(3)-O(5)#9	103.55(15)
B(6)-O(8)#9	1.397(9)	O(14)-Sr(3)-O(5)#9	51.13(14)
B(7)-O(18)	1.345(10)	O(10)-Sr(3)-O(5)#9	71.17(14)
B(7)-O(3)#4	1.358(10)	O(7)#8-Sr(3)-O(5)#9	86.09(14)
B(7)-O(4)	1.380(10)	O(17)#5-Sr(3)-O(5)#9	121.50(14)
B(8)-O(14)	1.351(9)	O(19)#7-Sr(3)-O(7)	158.3(3)
B(8)-O(13)	1.354(9)	O(9)-Sr(3)-O(7)	104.36(15)
B(8)-O(15)#9	1.383(9)	O(8)-Sr(3)-O(7)	71.19(15)
B(9)-O(6)#12	1.340(9)	O(11)-Sr(3)-O(7)	122.39(14)
B(9)-O(5)#12	1.368(9)	O(14)-Sr(3)-O(7)	50.85(14)
B(9)-O(8)	1.369(9)	O(10)-Sr(3)-O(7)	119.19(13)
B(10)-O(2)	1.348(10)	O(7)#8-Sr(3)-O(7)	74.33(15)
B(10)-O(1)#3	1.371(10)	O(17)#5-Sr(3)-O(7)	84.13(14)
B(10)-O(16)	1.381(9)	O(5)#9-Sr(3)-O(7)	50.31(13)
O(1)-B(10)#3	1.371(10)	O(19)#7-Sr(3)-O(27)#7	31.4(6)
O(1)-Sr(1)#3	2.560(6)	O(9)-Sr(3)-O(27)#7	85.0(4)
O(2)-B(5)#10	1.441(9)	O(8)-Sr(3)-O(27)#7	58.8(6)
O(3)-B(7)#4	1.358(10)	O(11)-Sr(3)-O(27)#7	96.5(5)
O(4)-Sr(1)#4	2.576(5)	O(14)-Sr(3)-O(27)#7	150.7(4)
O(5)-B(9)#12	1.368(9)	O(10)-Sr(3)-O(27)#7	113.0(6)

O(5)-Sr(3)#5	2.804(5)	O(7)#8-Sr(3)-O(27)#7	71.5(5)
O(6)-B(9)#12	1.340(9)	O(17)#5-Sr(3)-O(27)#7	78.2(4)
O(7)-B(2)#9	1.450(8)	O(5)#9-Sr(3)-O(27)#7	156.0(4)
O(7)-Sr(3)#8	2.780(5)	O(7)-Sr(3)-O(27)#7	127.0(6)
O(8)-B(6)#5	1.397(9)	O(24)-V(1)-O(26)	145.4(8)
O(9)-B(1)#8	1.474(9)	O(24)-V(1)-O(25)	57.0(7)
O(10)-Sr(2)#9	2.836(5)	O(26)-V(1)-O(25)	108.9(8)
O(12)-B(5)#5	1.497(9)	O(24)-V(1)-O(22)	106.7(7)
O(12)-Sr(2)#6	2.802(5)	O(26)-V(1)-O(22)	61.7(7)
O(13)-B(4)#11	1.488(9)	O(25)-V(1)-O(22)	50.8(6)
O(14)-B(2)#9	1.507(9)	O(24)-V(1)-O(21)	117.5(6)
O(15)-B(8)#5	1.383(9)	O(26)-V(1)-O(21)	47.1(6)
O(15)-B(3)#6	1.398(9)	O(25)-V(1)-O(21)	135.4(6)
O(16)-B(4)#10	1.484(9)	O(22)-V(1)-O(21)	105.0(5)
O(17)-Sr(3)#9	2.783(5)	O(24)-V(1)-O(4)	109.5(5)
O(17)-Sr(2)#9	2.798(5)	O(26)-V(1)-O(4)	105.1(6)
O(18)-B(2)#2	1.421(9)	O(25)-V(1)-O(4)	112.0(5)
O(19)-Sr(3)#10	2.449(11)	O(22)-V(1)-O(4)	106.7(5)
O(20)-V(2)#1	1.874(11)	O(21)-V(1)-O(4)	110.9(4)
O(20)-Sr(1)#1	2.559(10)	O(24)-V(1)-O(21)#2	58.7(6)
O(21)-V(1)#2	1.914(10)	O(26)-V(1)-O(21)#2	106.5(6)
O(23)-Sr(1)#1	2.445(14)	O(25)-V(1)-O(21)#2	108.8(6)
O(24)-Sr(1)#2	2.519(13)	O(22)-V(1)-O(21)#2	138.2(5)
O(27)-Sr(3)#10	2.88(4)	O(21)-V(1)-O(21)#2	61.6(6)
O(23)#1-Sr(1)-O(24)#2	62.4(4)	O(4)-V(1)-O(21)#2	115.1(4)
O(23)#1-Sr(1)-O(26)	92.0(5)	O(23)-V(2)-O(28)	146.1(9)
O(24)#2-Sr(1)-O(26)	70.3(4)	O(23)-V(2)-O(27)	56.7(16)
O(23)#1-Sr(1)-O(28)	69.8(6)	O(28)-V(2)-O(27)	112.2(18)
O(24)#2-Sr(1)-O(28)	93.7(5)	O(23)-V(2)-O(19)	110.7(7)
O(26)-Sr(1)-O(28)	160.2(5)	O(28)-V(2)-O(19)	58.7(10)
O(23)#1-Sr(1)-O(20)#1	37.2(4)	O(27)-V(2)-O(19)	56.1(16)
O(24)#2-Sr(1)-O(20)#1	79.7(4)	O(23)-V(2)-O(1)	109.8(6)
O(26)-Sr(1)-O(20)#1	129.2(4)	O(28)-V(2)-O(1)	104.1(8)
O(28)-Sr(1)-O(20)#1	32.8(5)	O(27)-V(2)-O(1)	109.8(7)
O(23)#1-Sr(1)-O(1)#3	122.6(4)	O(19)-V(2)-O(1)	106.5(5)
O(24)#2-Sr(1)-O(1)#3	150.8(4)	O(23)-V(2)-O(20)	55.1(6)
O(26)-Sr(1)-O(1)#3	133.4(4)	O(28)-V(2)-O(20)	107.0(9)
O(28)-Sr(1)-O(1)#3	65.8(5)	O(27)-V(2)-O(20)	105.1(13)
O(20)#1-Sr(1)-O(1)#3	90.9(3)	O(19)-V(2)-O(20)	134.8(6)
O(23)#1-Sr(1)-O(3)	96.5(4)	O(1)-V(2)-O(20)	118.7(4)
O(24)#2-Sr(1)-O(3)	128.2(4)	O(23)-V(2)-O(20)#1	115.3(6)
O(26)-Sr(1)-O(3)	63.4(4)	O(28)-V(2)-O(20)#1	48.4(9)
O(28)-Sr(1)-O(3)	124.4(5)	O(27)-V(2)-O(20)#1	138.4(9)
O(20)#1-Sr(1)-O(3)	112.5(3)	O(19)-V(2)-O(20)#1	103.1(5)

O(1)#3-Sr(1)-O(3)	80.97(18)	O(1)-V(2)-O(20)#1	110.8(4)
O(23)#1-Sr(1)-O(4)#4	148.0(4)	O(20)-V(2)-O(20)#1	61.8(5)
O(24)#2-Sr(1)-O(4)#4	123.7(3)	O(7)-B(1)-O(3)	111.3(6)
O(26)-Sr(1)-O(4)#4	65.7(4)	O(7)-B(1)-O(9)#8	107.7(6)
O(28)-Sr(1)-O(4)#4	134.1(5)	O(3)-B(1)-O(9)#8	109.1(6)
O(20)#1-Sr(1)-O(4)#4	156.5(3)	O(7)-B(1)-O(6)	111.3(6)
O(1)#3-Sr(1)-O(4)#4	69.2(2)	O(3)-B(1)-O(6)	108.4(6)
O(3)-Sr(1)-O(4)#4	53.77(16)	O(9)#8-B(1)-O(6)	108.9(5)
O(23)#1-Sr(1)-O(16)	125.1(4)	O(18)#2-B(2)-O(7)#5	114.6(6)
O(24)#2-Sr(1)-O(16)	98.5(4)	O(18)#2-B(2)-O(5)	110.6(6)
O(26)-Sr(1)-O(16)	131.8(4)	O(7)#5-B(2)-O(5)	109.1(6)
O(28)-Sr(1)-O(16)	60.3(5)	O(18)#2-B(2)-O(14)#5	109.7(6)
O(20)#1-Sr(1)-O(16)	91.8(3)	O(7)#5-B(2)-O(14)#5	107.3(5)
O(1)#3-Sr(1)-O(16)	53.86(16)	O(5)-B(2)-O(14)#5	105.0(5)
O(3)-Sr(1)-O(16)	129.40(17)	O(12)-B(3)-O(11)	125.4(7)
O(4)#4-Sr(1)-O(16)	86.40(18)	O(12)-B(3)-O(15)#6	114.9(6)
O(23)#1-Sr(1)-O(21)	79.0(4)	O(11)-B(3)-O(15)#6	119.5(6)
O(24)#2-Sr(1)-O(21)	39.5(4)	O(10)-B(4)-O(11)	106.7(6)
O(26)-Sr(1)-O(21)	30.9(4)	O(10)-B(4)-O(16)#7	112.1(6)
O(28)-Sr(1)-O(21)	132.7(5)	O(11)-B(4)-O(16)#7	108.5(5)
O(20)#1-Sr(1)-O(21)	111.0(3)	O(10)-B(4)-O(13)#11	112.4(5)
O(1)#3-Sr(1)-O(21)	157.9(3)	O(11)-B(4)-O(13)#11	109.2(5)
O(3)-Sr(1)-O(21)	92.9(3)	O(16)#7-B(4)-O(13)#11	107.9(6)
O(4)#4-Sr(1)-O(21)	90.0(3)	O(2)#7-B(5)-O(10)	112.1(6)
O(16)-Sr(1)-O(21)	119.8(3)	O(2)#7-B(5)-O(17)	108.9(6)
O(22)-Sr(2)-O(13)	81.8(3)	O(10)-B(5)-O(17)	110.0(6)
O(22)-Sr(2)-O(15)	91.1(3)	O(2)#7-B(5)-O(12)#9	112.0(6)
O(13)-Sr(2)-O(15)	118.87(15)	O(10)-B(5)-O(12)#9	106.1(5)
O(22)-Sr(2)-O(6)	71.6(3)	O(17)-B(5)-O(12)#9	107.5(5)
O(13)-Sr(2)-O(6)	115.98(16)	O(17)-B(6)-O(9)	125.7(7)
O(15)-Sr(2)-O(6)	118.77(16)	O(17)-B(6)-O(8)#9	114.6(6)
O(22)-Sr(2)-O(25)	31.4(4)	O(9)-B(6)-O(8)#9	119.6(6)
O(13)-Sr(2)-O(25)	81.7(3)	O(18)-B(7)-O(3)#4	123.3(7)
O(15)-Sr(2)-O(25)	64.7(3)	O(18)-B(7)-O(4)	120.3(7)
O(6)-Sr(2)-O(25)	99.6(3)	O(3)#4-B(7)-O(4)	116.4(7)
O(22)-Sr(2)-O(5)	89.1(3)	O(14)-B(8)-O(13)	117.8(6)
O(13)-Sr(2)-O(5)	167.00(16)	O(14)-B(8)-O(15)#9	123.0(6)
O(15)-Sr(2)-O(5)	70.33(15)	O(13)-B(8)-O(15)#9	119.2(7)
O(6)-Sr(2)-O(5)	51.82(14)	O(6)#12-B(9)-O(5)#12	116.9(7)
O(25)-Sr(2)-O(5)	95.4(3)	O(6)#12-B(9)-O(8)	120.5(7)
O(22)-Sr(2)-O(17)#5	138.7(3)	O(5)#12-B(9)-O(8)	122.4(6)
O(13)-Sr(2)-O(17)#5	99.94(15)	O(2)-B(10)-O(1)#3	121.1(7)
O(15)-Sr(2)-O(17)#5	121.86(15)	O(2)-B(10)-O(16)	123.2(7)

O(6)-Sr(2)-O(17)#5	70.68(15)	O(1)#3-B(10)-O(16)	115.7(7)
O(25)-Sr(2)-O(17)#5	169.9(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z #2 -x+1,-y+1,-z #3 -x,-y+2,-z #4 -x,-y+1,-z #5 x+1,y,z #6 -x+1,-y+1,-z+1 #7 x,y,z+1 #8 -x,-y+2,-z+1 #9 x-1,y,z #10 x,y,z-1 #11 -x,-y+1,-z+1 #12 -x+1,-y+2,-z+1

Fig. S1 The structural environments of (a) the Sr atoms and (b) the Ca atoms.

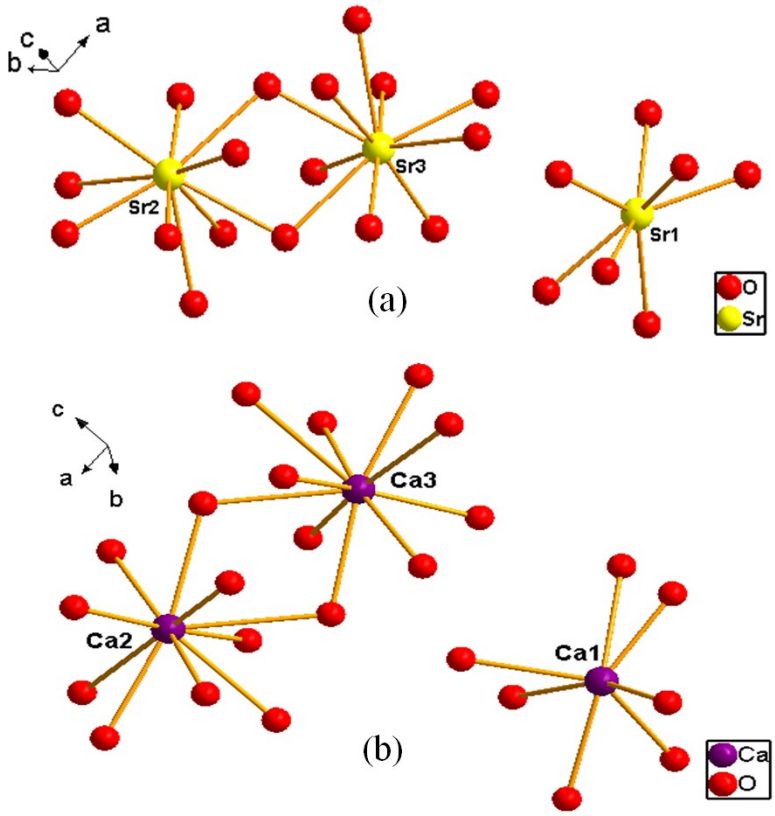

Fig. S2 The IR spectra of (a) $Ca_3V_2B_{10}O_{23}$ and (b) $Sr_3V_2B_{10}O_{23}$.

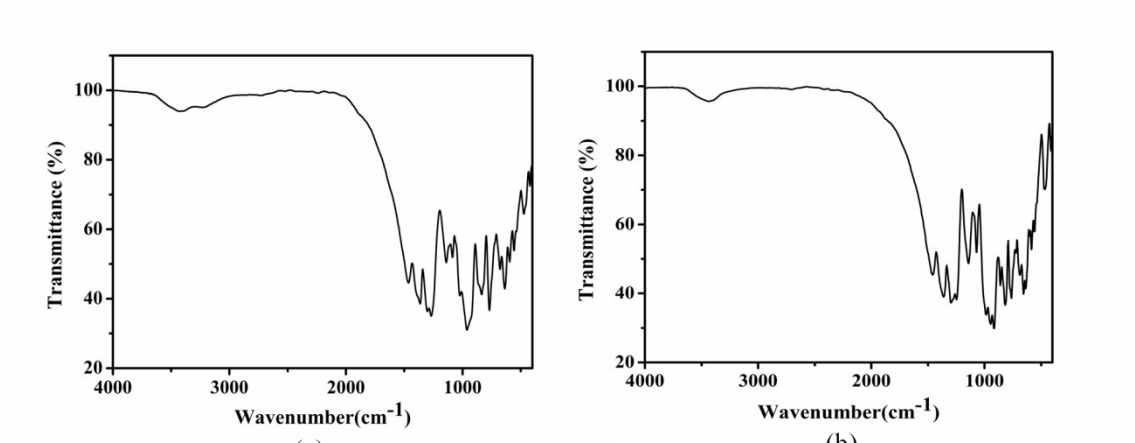
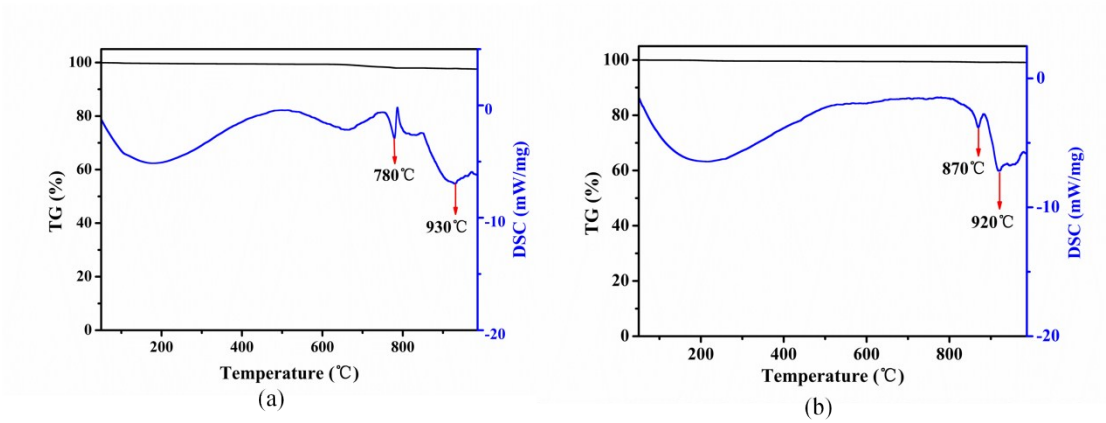
Fig. S3 The TG and DSC curves of (a) $Ca_3V_2B_{10}O_{23}$ and (b) $Sr_3V_2B_{10}O_{23}$.