Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information

$Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$: A New UV Nonlinear Optical Material with $[B_{10}O_{23}]^{16-}$ Building Block

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Table S1. Selected bond lengths (Å) and bond angles (deg) for $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$.[a]

Sr(1)-O(21)#1	2.497(4)	O(18)-Sr(2)-O(17)#4	118.69(12)
Sr(1)-O(2)	2.540(4)	O(6)#4-Sr(2)-O(17)#4	64.71(11)
Sr(1)-O(22)	2.550(4)	O(15)-Sr(2)-O(17)#4	117.74(11)
Sr(1)-O(9)	2.554(4)	O(20)#5-Sr(2)-O(17)#4	72.74(11)
Sr(1)-O(12)	2.598(4)	O(3)-Sr(2)-O(17)#4	50.09(11)
Sr(1)-O(1)	2.652(4)	O(10)-Sr(2)-O(17)#4	66.97(11)
Sr(1)-O(19)	2.737(4)	O(4)#5-Sr(2)-O(17)#4	146.27(12)
Sr(1)-O(16)	2.841(4)	O(2)#8-Sr(3)-O(13)	158.06(15)
Sr(2)-O(18)	2.564(4)	O(2)#8-Sr(3)-O(14)	83.64(12)
Sr(2)-O(13)	2.581(5)	O(13)-Sr(3)-O(14)	78.89(13)
Sr(2)-O(6)#4	2.601(4)	O(2)#8-Sr(3)-O(11)	95.01(12)
Sr(2)-O(15)	2.612(4)	O(13)-Sr(3)-O(11)	82.48(12)
Sr(2)-O(20)#5	2.615(4)	O(14)-Sr(3)-O(11)	119.88(12)
Sr(2)-O(3)	2.641(3)	O(2)#8-Sr(3)-O(3)	84.88(12)
Sr(2)-O(10)	2.679(4)	O(13)-Sr(3)-O(3)	74.12(12)
Sr(2)-O(4)#5	2.835(3)	O(14)-Sr(3)-O(3)	53.74(11)
Sr(2)-O(17)#4	2.883(4)	O(11)-Sr(3)-O(3)	66.24(11)
Sr(3)-O(2)#8	2.557(4)	O(2)#8-Sr(3)-O(8)	84.99(12)
Sr(3)-O(13)	2.581(4)	O(13)-Sr(3)-O(8)	109.36(13)
Sr(3)-O(14)	2.606(4)	O(14)-Sr(3)-O(8)	164.59(11)
Sr(3)-O(11)	2.631(4)	O(11)-Sr(3)-O(8)	50.94(11)
Sr(3)-O(3)	2.637(4)	O(3)-Sr(3)-O(8)	114.85(10)
Sr(3)-O(8)	2.646(4)	O(2)#8-Sr(3)-O(1)#8	74.11(12)
Sr(3)-O(1)#8	2.661(4)	O(13)-Sr(3)-O(1)#8	125.91(12)
Sr(3)-O(12)	2.665(4)	O(14)-Sr(3)-O(1)#8	117.05(11)
Sr(3)-O(16)	2.960(4)	O(11)-Sr(3)-O(1)#8	120.14(11)
Sr(4)-O(20)	2.492(4)	O(3)-Sr(3)-O(1)#8	158.30(11)
Sr(4)-O(22)	2.511(4)	O(8)-Sr(3)-O(1)#8	69.35(11)
Sr(4)-O(5)	2.521(4)	O(2)#8-Sr(3)-O(12)	92.38(12)
Sr(4)-O(7)	2.541(3)	O(13)-Sr(3)-O(12)	93.87(12)
Sr(4)-O(6)	2.580(4)	O(14)-Sr(3)-O(12)	69.65(12)
Sr(4)-O(19)	2.704(4)	O(11)-Sr(3)-O(12)	168.53(12)
Sr(4)-O(4)	2.750(4)	O(3)-Sr(3)-O(12)	123.31(11)
Sr(4)-O(17)	2.821(4)	O(8)-Sr(3)-O(12)	121.29(12)
B(1)-O(18)	1.366(7)	O(1)#8-Sr(3)-O(12)	53.86(11)
B(1)-O(15)#1	1.368(7)	O(2)#8-Sr(3)-O(16)	122.31(12)
B(1)-O(10)#1	1.375(7)	O(13)-Sr(3)-O(16)	79.16(12)
B(2)-O(4)	1.442(7)	O(14)-Sr(3)-O(16)	126.51(11)
B(2)-O(3)#10	1.481(7)	O(11)-Sr(3)-O(16)	104.62(11)
B(2)-O(18)#9	1.487(6)	O(3)-Sr(3)-O(16)	152.60(10)
B(2)-O(17)#1	1.495(7)	O(8)-Sr(3)-O(16)	68.64(11)

B(3)-O(6)#5	1.449(7)	O(1)#8-Sr(3)-O(16)	48.98(10)
B(3)-O(3)#11	1.475(7)	O(12)-Sr(3)-O(16)	63.95(11)
B(3)-O(15)	1.484(7)	O(20)-Sr(4)-O(22)	156.55(14)
B(3)-O(14)#11	1.496(7)	O(20)-Sr(4)-O(5)	91.21(13)
B(4)-O(5)	1.337(7)	O(22)-Sr(4)-O(5)	95.68(12)
B(4)-O(17)#1	1.375(7)	O(20)-Sr(4)-O(7)	81.45(12)
B(4)-O(7)#1	1.381(7)	O(22)-Sr(4)-O(7)	76.05(13)
B(5)-O(21)	1.358(7)	O(5)-Sr(4)-O(7)	123.54(12)
B(5)-O(9)	1.362(7)	O(20)-Sr(4)-O(6)	110.31(13)
B(5)-O(16)	1.386(7)	O(22)-Sr(4)-O(6)	86.11(13)
B(6)-O(14)	1.358(7)	O(5)-Sr(4)-O(6)	117.95(12)
B(6)-O(11)#1	1.360(7)	O(7)-Sr(4)-O(6)	117.02(12)
B(6)-O(8)#1	1.369(7)	O(20)-Sr(4)-O(19)	88.12(12)
B(7)-O(19)	1.453(7)	O(22)-Sr(4)-O(19)	78.28(12)
B(7)-O(1)#2	1.456(7)	O(5)-Sr(4)-O(19)	53.29(11)
B(7)-O(16)#1	1.493(7)	O(7)-Sr(4)-O(19)	70.49(11)
B(7)-O(5)	1.517(7)	O(6)-Sr(4)-O(19)	160.57(11)
B(8)-O(10)#10	1.457(7)	O(20)-Sr(4)-O(4)	79.98(12)
B(8)-O(4)	1.462(7)	O(22)-Sr(4)-O(4)	123.44(12)
B(8)-O(6)	1.478(7)	O(5)-Sr(4)-O(4)	75.81(11)
B(8)-O(11)#10	1.484(7)	O(7)-Sr(4)-O(4)	153.41(11)
B(9)-O(1)#6	1.454(7)	O(6)-Sr(4)-O(4)	53.78(12)
B(9)-O(12)#11	1.466(7)	O(19)-Sr(4)-O(4)	127.43(11)
B(9)-O(7)#11	1.478(7)	O(20)-Sr(4)-O(17)	99.36(13)
B(9)-O(21)	1.501(7)	O(22)-Sr(4)-O(17)	71.45(12)
B(10)-O(8)	1.462(7)	O(5)-Sr(4)-O(17)	166.67(11)
B(10)-O(19)#6	1.468(7)	O(7)-Sr(4)-O(17)	51.13(11)
B(10)-O(9)#8	1.473(7)	O(6)-Sr(4)-O(17)	65.89(11)
B(10)-O(12)#6	1.483(7)	O(19)-Sr(4)-O(17)	118.56(10)
O(21)#1-Sr(1)-O(2)	81.27(13)	O(4)-Sr(4)-O(17)	113.87(11)
O(21)#1-Sr(1)-O(22)	74.05(13)	O(18)-B(1)-O(15)#1	120.3(5)
O(2)-Sr(1)-O(22)	153.76(13)	O(18)-B(1)-O(10)#1	123.3(5)
O(21)#1-Sr(1)-O(9)	122.04(11)	O(15)#1-B(1)-O(10)#1	116.2(5)
O(2)-Sr(1)-O(9)	83.60(13)	O(4)-B(2)-O(3)#10	115.1(5)
O(22)-Sr(1)-O(9)	101.91(13)	O(4)-B(2)-O(18)#9	104.8(4)
O(21)#1-Sr(1)-O(12)	123.89(12)	O(3)#10-B(2)-O(18)#9	110.1(4)
O(2)-Sr(1)-O(12)	96.79(13)	O(4)-B(2)-O(17)#1	114.4(4)
O(22)-Sr(1)-O(12)	104.21(13)	O(3)#10-B(2)-O(17)#1	104.2(4)
O(9)-Sr(1)-O(12)	113.28(11)	O(18)#9-B(2)-O(17)#1	108.3(4)
O(21)#1-Sr(1)-O(1)	54.45(11)	O(6)#5-B(3)-O(3)#11	111.5(4)
O(2)-Sr(1)-O(1)	74.53(12)	O(6)#5-B(3)-O(15)	110.3(5)
O(22)-Sr(1)-O(1)	83.83(12)	O(3)#11-B(3)-O(15)	110.5(4)
O(9)-Sr(1)-O(1)	67.60(11)	O(6)#5-B(3)-O(14)#11	110.4(4)

O(12)-Sr(1)-O(1)	171.23(12)	O(3)#11-B(3)-O(14)#11	105.8(5)
O(21)#1-Sr(1)-O(19)	72.95(11)	O(15)-B(3)-O(14)#11	108.2(4)
O(2)-Sr(1)-O(19)	104.33(12)	O(5)-B(4)-O(17)#1	124.0(5)
O(22)-Sr(1)-O(19)	77.02(12)	O(5)-B(4)-O(7)#1	120.6(5)
O(9)-Sr(1)-O(19)	164.41(10)	O(17)#1-B(4)-O(7)#1	115.2(5)
O(12)-Sr(1)-O(19)	53.08(10)	O(21)-B(5)-O(9)	122.5(5)
O(1)-Sr(1)-O(19)	127.17(11)	O(21)-B(5)-O(16)	122.5(5)
O(21)#1-Sr(1)-O(16)	166.63(12)	O(9)-B(5)-O(16)	115.0(5)
O(2)-Sr(1)-O(16)	106.98(12)	O(14)-B(6)-O(11)#1	123.7(5)
O(22)-Sr(1)-O(16)	95.84(12)	O(14)-B(6)-O(8)#1	123.8(5)
O(9)-Sr(1)-O(16)	50.53(10)	O(11)#1-B(6)-O(8)#1	112.5(5)
O(12)-Sr(1)-O(16)	66.50(11)	O(19)-B(7)-O(1)#2	114.4(5)
O(1)-Sr(1)-O(16)	116.73(11)	O(19)-B(7)-O(16)#1	114.8(4)
O(19)-Sr(1)-O(16)	113.90(10)	O(1)#2-B(7)-O(16)#1	105.4(4)
O(18)-Sr(2)-O(6)#4	72.30(11)	O(19)-B(7)-O(5)	104.5(4)
O(18)-Sr(2)-O(15)	115.72(11)	O(1)#2-B(7)-O(5)	110.3(4)
O(6)#4-Sr(2)-O(15)	163.79(12)	O(16)#1-B(7)-O(5)	107.4(4)
O(18)-Sr(2)-O(20)#5	94.54(13)	O(10)#10-B(8)-O(4)	106.9(4)
O(6)#4-Sr(2)-O(20)#5	119.44(13)	O(10)#10-B(8)-O(6)	110.2(4)
O(15)-Sr(2)-O(20)#5	75.16(13)	O(4)-B(8)-O(6)	110.5(4)
O(18)-Sr(2)-O(3)	125.85(11)	O(10)#10-B(8)-O(11)#10	109.0(4)
O(6)#4-Sr(2)-O(3)	54.92(10)	O(4)-B(8)-O(11)#10	111.8(4)
O(15)-Sr(2)-O(3)	112.98(11)	O(6)-B(8)-O(11)#10	108.6(4)
O(20)#5-Sr(2)-O(3)	119.85(12)	O(1)#6-B(9)-O(12)#11	111.4(5)
O(18)-Sr(2)-O(10)	161.60(12)	O(1)#6-B(9)-O(7)#11	110.5(5)
O(6)#4-Sr(2)-O(10)	123.32(11)	O(12)#11-B(9)-O(7)#11	111.1(4)
O(15)-Sr(2)-O(10)	52.22(11)	O(1)#6-B(9)-O(21)	105.9(4)
O(20)#5-Sr(2)-O(10)	69.76(12)	O(12)#11-B(9)-O(21)	109.9(5)
O(3)-Sr(2)-O(10)	71.87(10)	O(7)#11-B(9)-O(21)	107.9(5)
O(18)-Sr(2)-O(4)#5	50.61(11)	O(8)-B(10)-O(19)#6	106.7(4)
O(6)#4-Sr(2)-O(4)#5	122.45(10)	O(8)-B(10)-O(9)#8	108.1(4)
O(15)-Sr(2)-O(4)#5	65.48(10)	O(19)#6-B(10)-O(9)#8	112.9(4)
O(20)#5-Sr(2)-O(4)#5	76.38(12)	O(8)-B(10)-O(12)#6	110.5(5)
O(3)-Sr(2)-O(4)#5	163.37(11)	O(19)#6-B(10)-O(12)#6	108.0(5)
O(10)-Sr(2)-O(4)#5	114.13(10)	O(9)#8-B(10)-O(12)#6	110.6(4)
	Numerical Refined Hydrogen Bonding		
O(2)···O(13)	2.4611	O(2)-H(1)-O(13)	177.058
O(13)···O(14)#6	3.3581	O(13)-H(2)-O(14)#6	158.662
O(2)···O(11)#1	3.6702	O(2)-H(3)-O(11)#1	149.925
O(20)···O(22)#2	2.4342	O(20)-H(4)-O(22)#2	174.420
O(20)···O(21)#2	3.2980	O(20)-H(5)-O(21)#2	146.405
O(22)#2··· O(7)#1	3.6000	O(22)#2-H(6)-O(7)#1	149.512

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

Table S2. Anisotropic displacement parameters for $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$.

	U11	U22	U33	U23	U13	U12
Sr(1)	8(1)	10(1)	20(1)	0(1)	-3(1)	-3(1)
Sr(2)	9(1)	9(1)	19(1)	-1(1)	1(1)	-3(1)
Sr(3)	14(1)	11(1)	10(1)	0(1)	-1(1)	-6(1)
Sr(4)	15(1)	10(1)	11(1)	1(1)	-3(1)	-5(1)
B(1)	11(3)	10(3)	11(3)	-1(3)	3(3)	-6(3)
B(2)	4(3)	4(3)	11(3)	-1(2)	1(2)	0(2)
B(3)	7(3)	5(3)	15(3)	-1(3)	-7(2)	0(2)
B(4)	7(3)	15(3)	7(3)	2(3)	-3(2)	-5(3)
B(5)	11(3)	6(3)	10(3)	-4(2)	-1(2)	2(3)
B(6)	13(3)	6(3)	14(3)	2(3)	-7(3)	-1(3)
B(7)	8(3)	8(3)	10(3)	-2(2)	-1(2)	-3(3)
B(8)	6(3)	3(3)	10(3)	0(2)	-5(2)	1(2)
B(9)	8(3)	12(3)	7(3)	5(3)	-4(2)	-5(3)
B(10)	8(3)	8(3)	7(3)	1(2)	-3(2)	-3(3)
O(1)	8(2)	7(2)	6(2)	0(2)	-4(2)	-1(2)
O(2)	16(2)	30(3)	18(3)	3(2)	-8(2)	-12(2)
O(3)	7(2)	4(2)	9(2)	1(2)	-3(2)	-3(2)
O(4)	6(2)	6(2)	12(2)	-1(2)	-3(2)	-1(2)
O(5)	18(2)	10(2)	8(2)	1(2)	-5(2)	-7(2)
O(6)	8(2)	8(2)	9(2)	3(2)	-4(2)	-3(2)
O(7)	19(2)	9(2)	5(2)	3(2)	-6(2)	-6(2)
O(8)	15(2)	9(2)	7(2)	-1(2)	-2(2)	-6(2)
O(9)	7(2)	7(2)	17(2)	3(2)	-2(2)	-3(2)
O(10)	7(2)	7(2)	14(2)	4(2)	-3(2)	-3(2)
O(11)	16(2)	15(2)	7(2)	0(2)	-1(2)	-8(2)
O(12)	8(2)	5(2)	13(2)	-1(2)	0(2)	-3(2)
O(13)	13(2)	26(2)	27(3)	1(2)	-3(2)	-5(2)
O(14)	16(2)	11(2)	8(2)	-1(2)	0(2)	-8(2)
O(15)	7(2)	8(2)	21(2)	3(2)	-8(2)	-2(2)
O(16)	5(2)	9(2)	22(2)	3(2)	-2(2)	-2(2)
O(17)	17(2)	12(2)	9(2)	0(2)	-3(2)	-7(2)
O(18)	8(2)	10(2)	22(2)	2(2)	-4(2)	-5(2)
O(19)	9(2)	6(2)	9(2)	2(2)	-6(2)	-3(2)
O(20)	16(2)	20(2)	21(3)	-2(2)	-5(2)	-4(2)
O(21)	5(2)	7(2)	19(2)	2(2)	-1(2)	-1(2)
O(22)	14(2)	17(2)	26(3)	4(2)	-2(2)	-4(2)

Table S3. The SHG coefficients (d_{in}) for $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$ and $Sr_2B_5O_9OH \cdot H_2O$ obtained by DFT method.

d_{in} (pm/V)	d_{11}	d_{16}	d_{15}	d_{12}	d_{14}	d_{13}	d_{22}	d_{24}	d_{23}	d_{33}
$Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$	0.92	− 0.48	0.52	0.56	0.03	0.36	0.91	0.56	0.57	0.86
$Sr_2B_5O_9OH \cdot H_2O$		1.05			− 0.81		− 0.37		− 0.74	

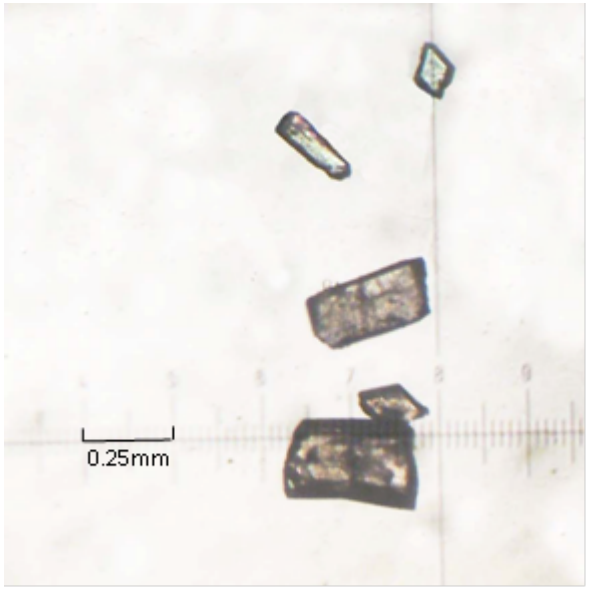

Figure S1. The crystal photograph of $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$.

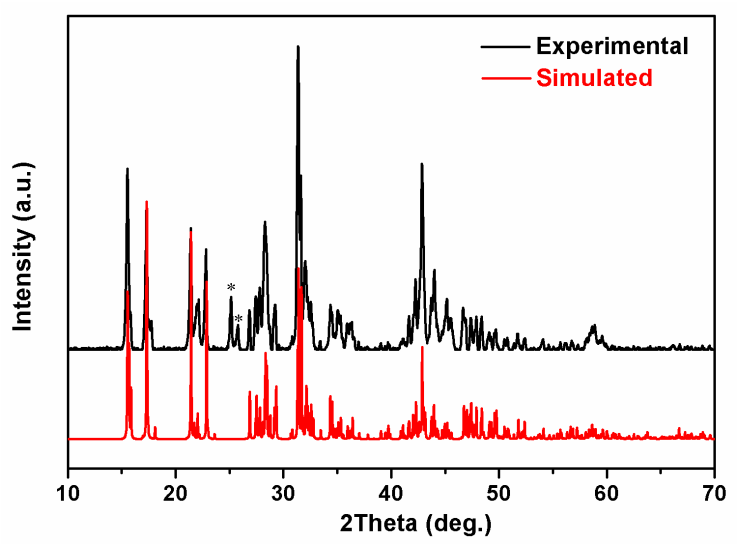

Figure S2. Powder XRD patterns of $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$.

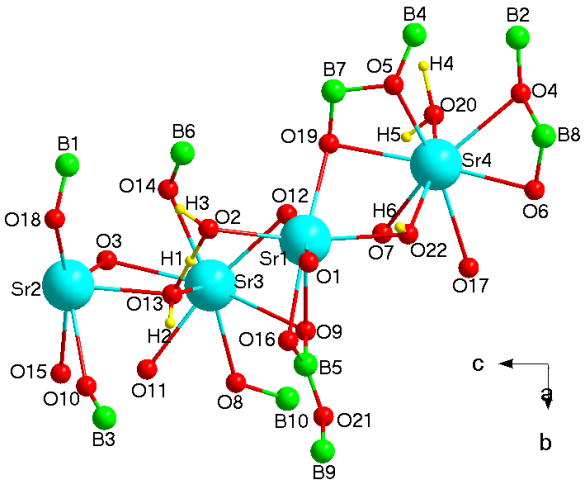

Figure S3. Asymmetric unit of $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$.

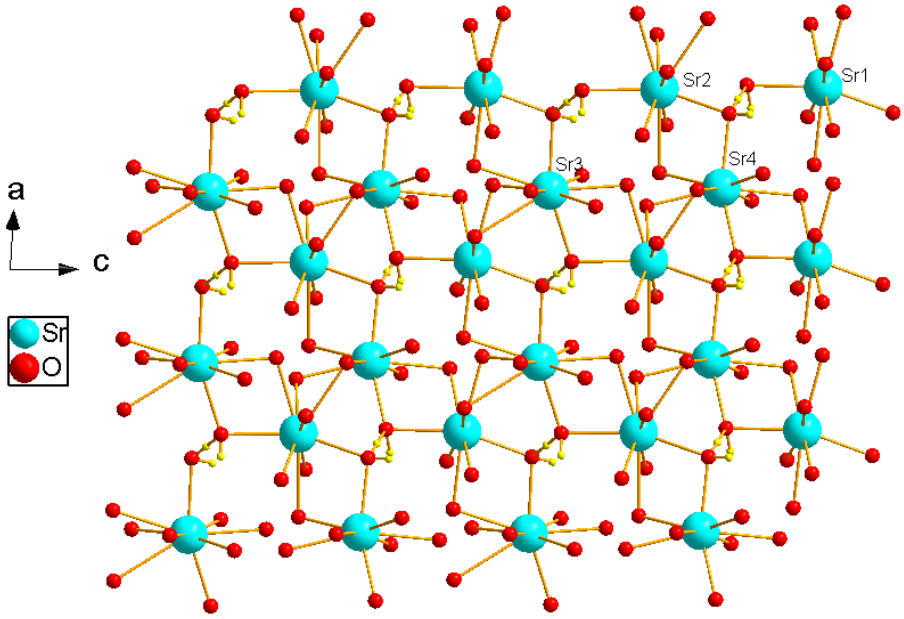

Figure S4. The network formed by the Sr-O groups.

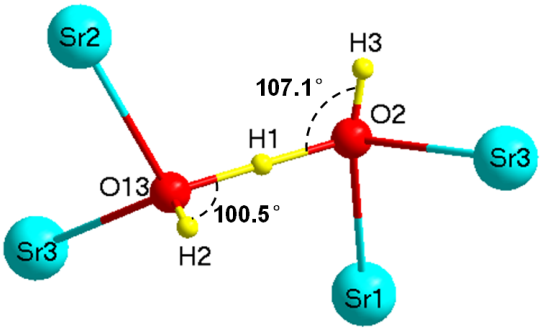

Figure S5. Coordination environments of O(2) and O(13).

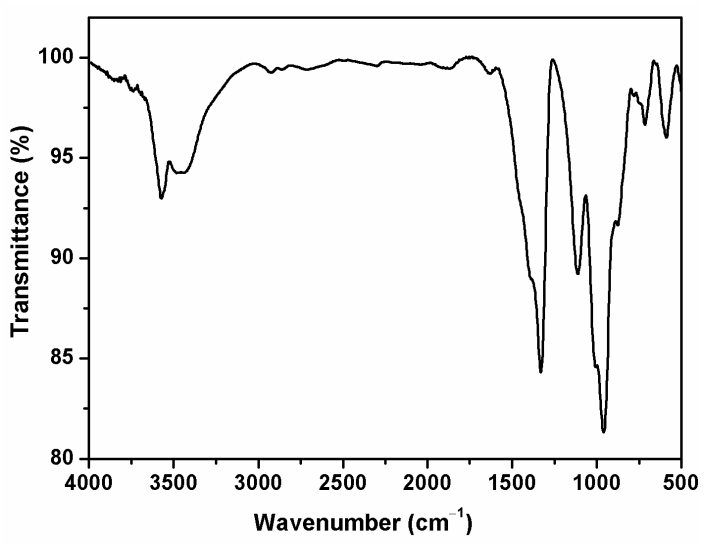

Figure S6. IR spectrum of $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$

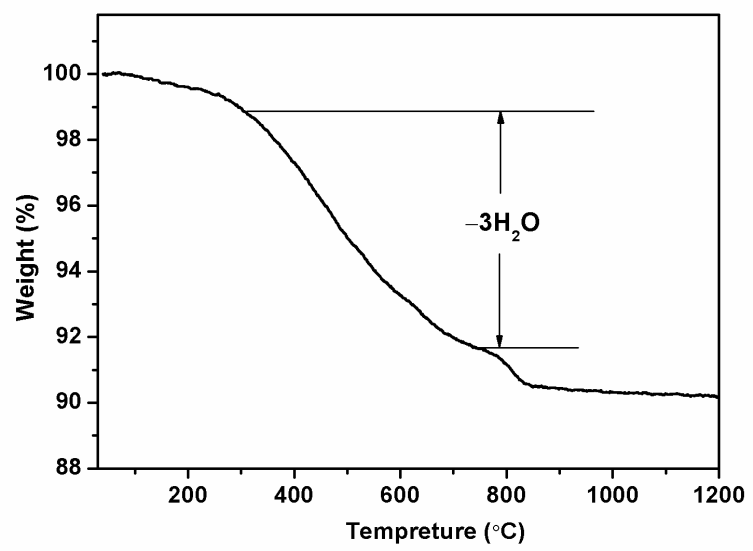

Figure S7. TGA curve of $Sr_4B_{10}O_{18}(OH)_2 \cdot 2H_2O$