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Supporting Information

$Sr_3B_{14}O_{24}$: A New Borate with $[B_{14}O_{30}]$ Fundamental Building Block and Unwonted 2D Double Layer

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Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$), and bond valence sum (BVS) calculations for $Sr_3B_{14}O_{24}$. *U*(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atoms	*x*/*a*	*y*/*b*	*z*/*c*	*U*(eq)	BVS
Sr(1)	17338(1)	894(1)	9443(1)	13(1)	2.20
Sr(2)	11795(1)	3308(1)	7312(1)	27(1)	1.97
Sr(3)	-2409(1)	832(1)	5561(1)	12(1)	2.27
B(1)	13910(10)	3314(6)	9300(3)	13(1)	3.05
B(2)	14570(11)	7040(6)	8132(4)	18(2)	3.05
B(3)	11615(11)	5912(6)	7925(3)	17(2)	3.10
B(4)	10306(10)	2865(5)	9055(3)	12(1)	3.04
B(5)	12788(10)	1334(6)	9321(3)	13(2)	3.04
B(6)	7354(9)	4220(5)	9143(3)	10(1)	3.04
B(7)	8461(10)	4758(6)	8116(3)	16(2)	3.06
B(8)	7275(10)	4686(6)	6949(3)	15(2)	3.07
B(9)	4117(10)	5906(6)	7177(3)	15(2)	3.01
B(10)	1056(11)	6981(6)	6931(3)	18(2)	3.02
B(11)	7669(10)	4168(5)	5836(3)	10(1)	3.05
B(12)	4532(10)	2889(6)	5851(3)	13(1)	3.07
B(13)	1000(9)	3329(6)	5572(3)	13(1)	3.06
B(14)	2172(10)	1340(6)	5589(3)	13(2)	3.02
O(1)	15693(6)	7828(3)	8478(2)	17(1)	2.03
O(2)	15168(6)	6822(3)	7564(2)	16(1)	1.98
O(3)	12929(6)	6550(3)	8371(2)	16(1)	2.12
O(4)	10218(6)	5320(4)	8298(2)	19(1)	1.93
O(5)	7072(6)	4453(3)	8501(2)	14(1)	1.95
O(6)	8450(5)	3184(3)	9312(2)	11(1)	1.91
O(7)	8237(6)	4461(4)	7504(2)	22(1)	2.15
O(8)	12885(6)	5194(3)	7560(2)	16(1)	2.09
O(9)	11955(6)	3664(3)	9226(2)	13(1)	2.08
O(10)	15330(6)	4140(3)	9406(2)	13(1)	2.06
O(11)	14320(5)	2154(3)	9295(2)	14(1)	2.29
O(12)	13422(5)	236(3)	9394(2)	13(1)	2.06
O(13)	10841(5)	1681(3)	9295(2)	13(1)	2.06
O(14)	8282(6)	4234(3)	6479(2)	16(1)	1.91
O(15)	6450(5)	3193(3)	5644(2)	12(1)	1.95
O(16)	4073(5)	1716(3)	5604(2)	13(1)	2.12
O(17)	2928(6)	3695(3)	5628(2)	13(1)	2.10
O(18)	603(5)	2153(3)	5620(2)	14(1)	2.17
O(19)	-461(5)	4128(3)	5492(2)	11(1)	2.14
O(20)	1591(5)	221(3)	5522(2)	12(1)	2.04
O(21)	5531(6)	5276(4)	6840(2)	22(1)	1.89
O(22)	2711(6)	6480(3)	6704(2)	17(1)	1.98
O(23)	521(6)	6752(3)	7514(2)	18(1)	2.17

O(24)	-201(6)	7742(3)	6620(2)	16(1)	1.95

Table S2. Anisotropic displacement parameters (Å^2) for $Sr_3B_{14}O_{24}$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sr(1)	10(1)	12(1)	16(1)	1(1)	-1(1)	-1(1)
Sr(2)	26(1)	18(1)	39(1)	-4(1)	15(1)	-5(1)
Sr(3)	9(1)	11(1)	16(1)	-2(1)	0(1)	0(1)
B(1)	14(3)	15(3)	9(4)	0(3)	2(3)	4(3)
B(2)	16(4)	17(4)	21(4)	2(3)	1(3)	-2(3)
B(3)	21(4)	17(4)	13(4)	3(3)	4(3)	-2(3)
B(4)	17(3)	5(3)	15(4)	5(3)	0(3)	2(2)
B(5)	11(3)	15(3)	13(4)	4(3)	3(3)	-7(3)
B(6)	7(3)	13(3)	11(4)	1(3)	1(3)	1(2)
B(7)	14(3)	15(4)	19(4)	3(3)	3(3)	9(3)
B(8)	17(3)	7(3)	21(4)	2(3)	4(3)	-5(3)
B(9)	17(3)	16(4)	15(4)	-4(3)	1(3)	1(3)
B(10)	20(4)	15(4)	18(4)	-4(3)	0(3)	-6(3)
B(11)	15(3)	6(3)	11(4)	0(3)	0(3)	2(3)
B(12)	10(3)	12(3)	15(4)	1(3)	-3(3)	-1(3)
B(13)	7(3)	15(3)	16(4)	1(3)	-2(3)	2(3)
B(14)	10(3)	9(3)	19(4)	1(3)	2(3)	1(2)
O(1)	19(2)	16(2)	15(2)	-3(2)	4(2)	-1(2)
O(2)	16(2)	21(2)	12(2)	-2(2)	5(2)	-4(2)
O(3)	20(2)	17(2)	12(2)	-4(2)	2(2)	-4(2)
O(4)	22(2)	20(2)	14(2)	1(2)	-2(2)	-7(2)
O(5)	12(2)	15(2)	15(2)	4(2)	-3(2)	0(2)
O(6)	11(2)	9(2)	12(2)	-1(2)	0(2)	-2(2)
O(7)	22(2)	26(2)	17(3)	0(2)	0(2)	4(2)
O(8)	18(2)	13(2)	16(2)	-2(2)	3(2)	-3(2)
O(9)	7(2)	10(2)	21(2)	0(2)	-2(2)	-2(2)
O(10)	11(2)	9(2)	19(2)	-2(2)	1(2)	0(2)
O(11)	10(2)	7(2)	25(3)	0(2)	2(2)	-2(2)
O(12)	7(2)	10(2)	20(2)	-1(2)	-1(2)	0(2)
O(13)	10(2)	11(2)	19(2)	4(2)	4(2)	1(2)
O(14)	18(2)	16(2)	13(2)	0(2)	0(2)	2(2)
O(15)	9(2)	10(2)	17(2)	-2(2)	0(2)	2(2)
O(16)	11(2)	5(2)	25(2)	-1(2)	0(2)	1(2)
O(17)	12(2)	5(2)	22(2)	0(2)	-1(2)	-1(2)
O(18)	8(2)	10(2)	24(3)	-1(2)	0(2)	1(2)
O(19)	9(2)	10(2)	14(2)	2(2)	2(2)	0(2)
O(20)	11(2)	6(2)	18(2)	1(2)	0(2)	1(2)
O(21)	20(2)	25(2)	23(3)	-7(2)	4(2)	7(2)
O(22)	16(2)	20(2)	13(2)	-3(2)	0(2)	7(2)
O(23)	20(2)	19(2)	15(2)	2(2)	2(2)	7(2)
O(24)	14(2)	13(2)	19(2)	3(2)	1(2)	2(2)

Table S3. Bond lengths (Å) and angles (°) for $Sr_3B_{14}O_{24}$.

Sr(1)-O(11)	2.489(4)	B(4)-O(6)	1.434(8)
Sr(1)-O(13)#1	2.540(4)	B(4)-O(9)	1.468(7)
Sr(1)-O(17)#2	2.565(4)	B(4)-O(24)#6	1.481(8)
Sr(1)-O(22)#2	2.601(4)	B(4)-O(13)	1.508(7)
Sr(1)-O(19)#3	2.651(4)	B(5)-O(12)	1.350(8)
Sr(1)-O(12)	2.709(4)	B(5)-O(13)	1.354(7)
Sr(1)-O(6)#1	2.780(4)	B(5)-O(11)	1.398(7)
Sr(1)-O(19)#2	2.917(4)	B(6)-O(5)	1.434(8)
Sr(1)-O(15)#4	2.928(4)	B(6)-O(6)	1.444(7)
Sr(1)-O(12)#5	2.935(4)	B(6)-O(10)#8	1.497(7)
Sr(2)-O(8)	2.362(4)	B(6)-O(20)#12	1.525(7)
Sr(2)-O(23)#6	2.419(4)	B(7)-O(5)	1.334(8)
Sr(2)-O(1)#7	2.535(4)	B(7)-O(4)	1.377(8)
Sr(2)-O(2)#7	2.659(4)	B(7)-O(7)	1.383(8)
Sr(2)-O(24)#6	2.704(4)	B(8)-O(21)	1.356(8)
Sr(2)-O(7)	2.771(4)	B(8)-O(14)	1.364(8)
Sr(2)-O(14)	3.074(4)	B(8)-O(7)	1.367(8)
Sr(3)-O(18)	2.521(4)	B(9)-O(21)	1.428(8)
Sr(3)-O(3)#6	2.526(4)	B(9)-O(8)#8	1.463(8)
Sr(3)-O(16)#8	2.561(4)	B(9)-O(2)#8	1.507(8)
Sr(3)-O(9)#6	2.577(4)	B(9)-O(22)	1.509(8)
Sr(3)-O(20)#9	2.749(4)	B(10)-O(22)	1.364(8)
Sr(3)-O(20)	2.759(4)	B(10)-O(23)	1.370(8)
Sr(3)-O(10)#6	2.768(4)	B(10)-O(24)	1.371(8)
Sr(3)-O(15)#8	2.855(4)	B(11)-O(15)	1.441(7)
Sr(3)-O(10)#10	2.865(4)	B(11)-O(14)	1.446(8)
Sr(3)-O(4)#6	2.881(4)	B(11)-O(19)#1	1.491(7)
Sr(3)-O(6)#11	3.049(4)	B(11)-O(12)#13	1.509(7)
B(1)-O(10)	1.357(8)	B(12)-O(15)	1.422(8)
B(1)-O(9)	1.363(7)	B(12)-O(17)	1.481(7)
B(1)-O(11)	1.376(8)	B(12)-O(1)#2	1.488(8)
B(2)-O(2)	1.352(9)	B(12)-O(16)	1.492(7)
B(2)-O(3)	1.361(8)	B(13)-O(19)	1.348(7)
B(2)-O(1)	1.380(8)	B(13)-O(17)	1.349(7)
B(3)-O(4)	1.445(8)	B(13)-O(18)	1.396(8)
B(3)-O(8)	1.458(8)	B(14)-O(16)	1.336(7)
B(3)-O(3)	1.473(8)	B(14)-O(20)	1.361(7)
B(3)-O(23)#1	1.489(8)	B(14)-O(18)	1.412(7)
O(11)-Sr(1)-O(13)#1	120.67(13)	O(6)-B(4)-O(9)	112.5(5)
O(11)-Sr(1)-O(17)#2	121.69(12)	O(6)-B(4)-O(24)#6	115.1(5)
O(13)#1-Sr(1)-O(17)#2	114.26(12)	O(9)-B(4)-O(24)#6	107.9(5)
O(11)-Sr(1)-O(22)#2	75.85(13)	O(6)-B(4)-O(13)	106.8(5)
O(13)#1-Sr(1)-O(22)#2	75.10(12)	O(9)-B(4)-O(13)	109.3(5)

O(17)#2-Sr(1)-O(22)#2	101.81(13)	O(24)#6-B(4)-O(13)	104.8(5)
O(11)-Sr(1)-O(19)#3	121.28(12)	O(12)-B(5)-O(13)	125.3(5)
O(13)#1-Sr(1)-O(19)#3	69.50(12)	O(12)-B(5)-O(11)	115.2(5)
O(17)#2-Sr(1)-O(19)#3	94.33(12)	O(13)-B(5)-O(11)	119.5(6)
O(22)#2-Sr(1)-O(19)#3	144.55(12)	O(5)-B(6)-O(6)	116.3(5)
O(11)-Sr(1)-O(12)	52.80(12)	O(5)-B(6)-O(10)#8	108.6(5)
O(13)#1-Sr(1)-O(12)	169.24(12)	O(6)-B(6)-O(10)#8	107.5(5)
O(17)#2-Sr(1)-O(12)	69.75(12)	O(5)-B(6)-O(20)#12	111.0(5)
O(22)#2-Sr(1)-O(12)	94.42(12)	O(6)-B(6)-O(20)#12	107.6(4)
O(19)#3-Sr(1)-O(12)	120.85(12)	O(10)#8-B(6)-O(20)#12	105.1(4)
O(11)-Sr(1)-O(6)#1	68.99(12)	O(5)-B(7)-O(4)	123.3(6)
O(13)#1-Sr(1)-O(6)#1	52.50(12)	O(5)-B(7)-O(7)	120.4(6)
O(17)#2-Sr(1)-O(6)#1	164.66(12)	O(4)-B(7)-O(7)	116.1(6)
O(22)#2-Sr(1)-O(6)#1	68.80(12)	O(21)-B(8)-O(14)	121.0(6)
O(19)#3-Sr(1)-O(6)#1	87.84(11)	O(21)-B(8)-O(7)	127.1(6)
O(12)-Sr(1)-O(6)#1	121.78(11)	O(14)-B(8)-O(7)	111.9(5)
O(11)-Sr(1)-O(19)#2	170.39(12)	O(21)-B(9)-O(8)#8	114.4(5)
O(13)#1-Sr(1)-O(19)#2	66.67(11)	O(21)-B(9)-O(2)#8	110.8(5)
O(17)#2-Sr(1)-O(19)#2	49.35(11)	O(8)#8-B(9)-O(2)#8	109.4(5)
O(22)#2-Sr(1)-O(19)#2	101.55(12)	O(21)-B(9)-O(22)	105.8(5)
O(19)#3-Sr(1)-O(19)#2	66.10(13)	O(8)#8-B(9)-O(22)	107.3(5)
O(12)-Sr(1)-O(19)#2	118.88(11)	O(2)#8-B(9)-O(22)	108.8(5)
O(6)#1-Sr(1)-O(19)#2	119.03(11)	O(22)-B(10)-O(23)	121.0(6)
O(11)-Sr(1)-O(15)#4	72.64(12)	O(22)-B(10)-O(24)	125.1(6)
O(13)#1-Sr(1)-O(15)#4	102.62(12)	O(23)-B(10)-O(24)	113.9(6)
O(17)#2-Sr(1)-O(15)#4	113.49(12)	O(15)-B(11)-O(14)	116.6(5)
O(22)#2-Sr(1)-O(15)#4	141.38(12)	O(15)-B(11)-O(19)#1	107.4(5)
O(19)#3-Sr(1)-O(15)#4	49.83(11)	O(14)-B(11)-O(19)#1	107.3(5)
O(12)-Sr(1)-O(15)#4	83.97(11)	O(15)-B(11)-O(12)#13	107.3(5)
O(6)#1-Sr(1)-O(15)#4	79.36(11)	O(14)-B(11)-O(12)#13	112.6(5)
O(19)#2-Sr(1)-O(15)#4	112.99(11)	O(19)#1-B(11)-O(12)#13	104.8(5)
O(11)-Sr(1)-O(12)#5	101.44(12)	O(15)-B(12)-O(17)	112.4(5)
O(13)#1-Sr(1)-O(12)#5	118.49(11)	O(15)-B(12)-O(1)#2	118.0(5)
O(17)#2-Sr(1)-O(12)#5	65.93(12)	O(17)-B(12)-O(1)#2	104.2(5)
O(22)#2-Sr(1)-O(12)#5	164.12(12)	O(15)-B(12)-O(16)	106.3(5)
O(19)#3-Sr(1)-O(12)#5	50.07(11)	O(17)-B(12)-O(16)	109.3(5)
O(12)-Sr(1)-O(12)#5	72.24(12)	O(1)#2-B(12)-O(16)	106.5(5)
O(6)#1-Sr(1)-O(12)#5	125.33(11)	O(19)-B(13)-O(17)	117.9(6)
O(19)#2-Sr(1)-O(12)#5	78.48(11)	O(19)-B(13)-O(18)	123.1(5)
O(15)#4-Sr(1)-O(12)#5	47.84(10)	O(17)-B(13)-O(18)	119.0(5)
O(8)-Sr(2)-O(23)#6	147.91(14)	O(16)-B(14)-O(20)	125.3(5)
O(8)-Sr(2)-O(1)#7	98.92(13)	O(16)-B(14)-O(18)	118.7(5)
O(23)#6-Sr(2)-O(1)#7	113.17(13)	O(20)-B(14)-O(18)	116.0(5)
O(8)-Sr(2)-O(2)#7	110.98(13)	O(20)#9-Sr(3)-O(15)#8	123.35(11)

O(23)#6-Sr(2)-O(2)#7	89.15(14)	O(10)#6-Sr(3)-O(15)#8	119.46(11)
O(1)#7-Sr(2)-O(2)#7	53.16(13)	O(18)-Sr(3)-O(10)#10	114.41(12)
O(8)-Sr(2)-O(24)#6	99.07(13)	O(3)#6-Sr(3)-O(10)#10	136.09(12)
O(23)#6-Sr(2)-O(24)#6	52.94(13)	O(16)#8-Sr(3)-O(10)#10	66.08(12)
O(1)#7-Sr(2)-O(24)#6	147.50(13)	O(9)#6-Sr(3)-O(10)#10	102.78(11)
O(2)#7-Sr(2)-O(24)#6	95.00(12)	O(20)#9-Sr(3)-O(10)#10	50.54(11)
O(8)-Sr(2)-O(7)	76.69(14)	O(20)-Sr(3)-O(10)#10	115.65(11)
O(23)#6-Sr(2)-O(7)	77.36(14)	O(10)#6-Sr(3)-O(10)#10	72.43(13)
O(1)#7-Sr(2)-O(7)	144.23(13)	O(15)#8-Sr(3)-O(10)#10	85.30(11)
O(2)#7-Sr(2)-O(7)	161.50(13)	O(18)-Sr(3)-O(4)#6	73.76(13)
O(24)#6-Sr(2)-O(7)	66.80(12)	O(3)#6-Sr(3)-O(4)#6	49.77(12)
O(8)-Sr(2)-O(14)	91.37(12)	O(16)#8-Sr(3)-O(4)#6	117.88(13)
O(23)#6-Sr(2)-O(14)	83.49(12)	O(9)#6-Sr(3)-O(4)#6	65.97(12)
O(1)#7-Sr(2)-O(14)	100.35(12)	O(20)#9-Sr(3)-O(4)#6	122.72(11)
O(2)#7-Sr(2)-O(14)	146.55(12)	O(20)-Sr(3)-O(4)#6	62.22(12)
O(24)#6-Sr(2)-O(14)	106.05(12)	O(10)#6-Sr(3)-O(4)#6	98.69(12)
O(7)-Sr(2)-O(14)	45.17(12)	O(15)#8-Sr(3)-O(4)#6	105.39(11)
O(18)-Sr(3)-O(3)#6	84.37(13)	O(10)#10-Sr(3)-O(4)#6	168.74(11)
O(18)-Sr(3)-O(16)#8	118.60(12)	O(18)-Sr(3)-O(6)#11	68.20(12)
O(3)#6-Sr(3)-O(16)#8	70.08(13)	O(3)#6-Sr(3)-O(6)#11	138.58(12)
O(18)-Sr(3)-O(9)#6	120.08(12)	O(16)#8-Sr(3)-O(6)#11	95.84(11)
O(3)#6-Sr(3)-O(9)#6	100.13(13)	O(9)#6-Sr(3)-O(6)#11	120.20(12)
O(16)#8-Sr(3)-O(9)#6	118.89(12)	O(20)#9-Sr(3)-O(6)#11	48.46(10)
O(18)-Sr(3)-O(20)#9	96.85(12)	O(20)-Sr(3)-O(6)#11	80.65(10)
O(3)#6-Sr(3)-O(20)#9	171.76(12)	O(10)#6-Sr(3)-O(6)#11	117.25(11)
O(16)#8-Sr(3)-O(20)#9	115.91(12)	O(15)#8-Sr(3)-O(6)#11	76.21(11)
O(9)#6-Sr(3)-O(20)#9	72.18(12)	O(10)#10-Sr(3)-O(6)#11	47.16(10)
O(18)-Sr(3)-O(20)	52.67(11)	O(4)#6-Sr(3)-O(6)#11	138.08(11)
O(3)#6-Sr(3)-O(20)	107.30(12)	O(20)-Sr(3)-O(15)#8	120.62(11)
O(16)#8-Sr(3)-O(20)	171.26(12)	O(10)-B(1)-O(9)	117.3(6)
O(9)#6-Sr(3)-O(20)	69.57(11)	O(10)-B(1)-O(11)	123.9(5)
O(20)#9-Sr(3)-O(20)	67.64(13)	O(9)-B(1)-O(11)	118.7(6)
O(18)-Sr(3)-O(10)#6	171.08(12)	O(2)-B(2)-O(3)	124.1(6)
O(3)#6-Sr(3)-O(10)#6	94.41(13)	O(2)-B(2)-O(1)	116.8(6)
O(16)#8-Sr(3)-O(10)#6	68.92(11)	O(3)-B(2)-O(1)	119.1(6)
O(9)#6-Sr(3)-O(10)#6	51.37(11)	O(4)-B(3)-O(8)	116.7(5)
O(20)#9-Sr(3)-O(10)#6	83.12(12)	O(4)-B(3)-O(3)	103.9(5)
O(20)-Sr(3)-O(10)#6	119.81(11)	O(8)-B(3)-O(3)	108.1(5)
O(18)-Sr(3)-O(15)#8	67.97(11)	O(4)-B(3)-O(23)#1	110.3(5)
O(3)#6-Sr(3)-O(15)#8	64.67(12)	O(8)-B(3)-O(23)#1	108.7(5)
O(16)#8-Sr(3)-O(15)#8	50.64(11)	O(3)-B(3)-O(23)#1	108.8(5)
O(9)#6-Sr(3)-O(15)#8	163.06(12)		

Symmetry transformations used to generate equivalent atoms:

#1 x + 1, y, z	#2 – x + 2, y – 1/2, –z + 3/2
#3 x + 2, – y + 1/2, z + 1/2	#4 x + 1, – y + 1/2, z + 1/2
#5 – x + 3, – y, – z + 2	#6 – x + 1, y – 1/2, – z + 3/2
#7 – x + 3, y – 1/2, – z + 3/2	#8 x – 1, y, z
#9 – x, – y, – z + 1	#10 x – 2, – y + 1/2, z – 1/2
#11 x – 1, – y + 1/2, z – 1/2	#12 –x + 1, y + 1/2, – z + 3/2
#13 – x + 2, y + 1/2, – z + 3/2	#14 – x + 3, y + 1/2, – z + 3/2

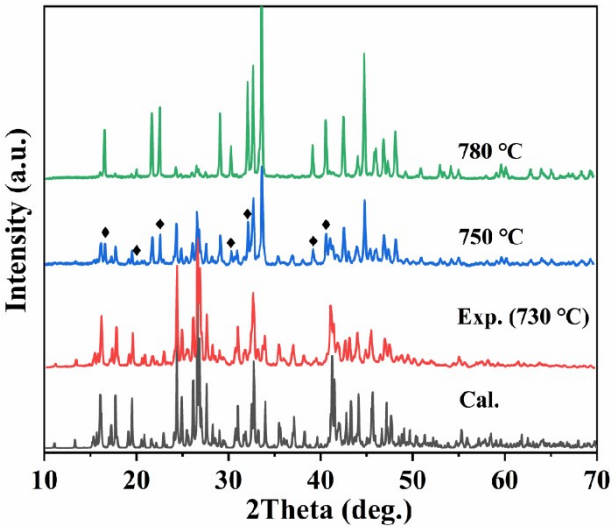
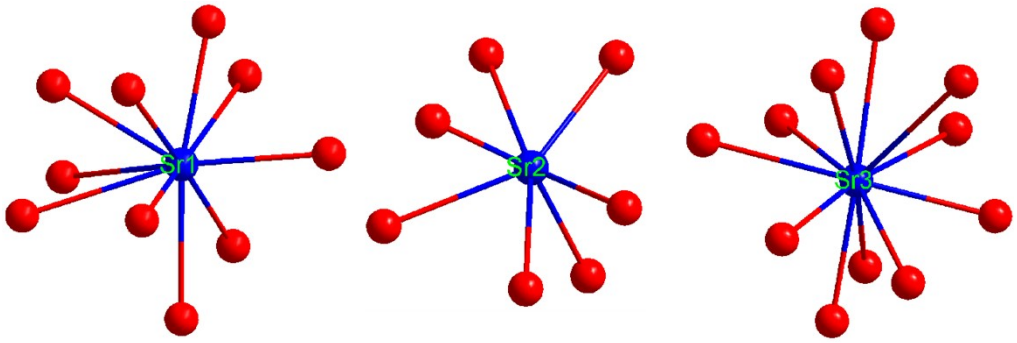


Fig. S1 Powder XRD patterns of $Sr_3B_{14}O_{24}$ after heating at different temperatures.



SrO_{10} SrO_7 SrO_{11}

Fig. S2 Coordination environments of the cations in $Sr_3B_{14}O_{24}$.

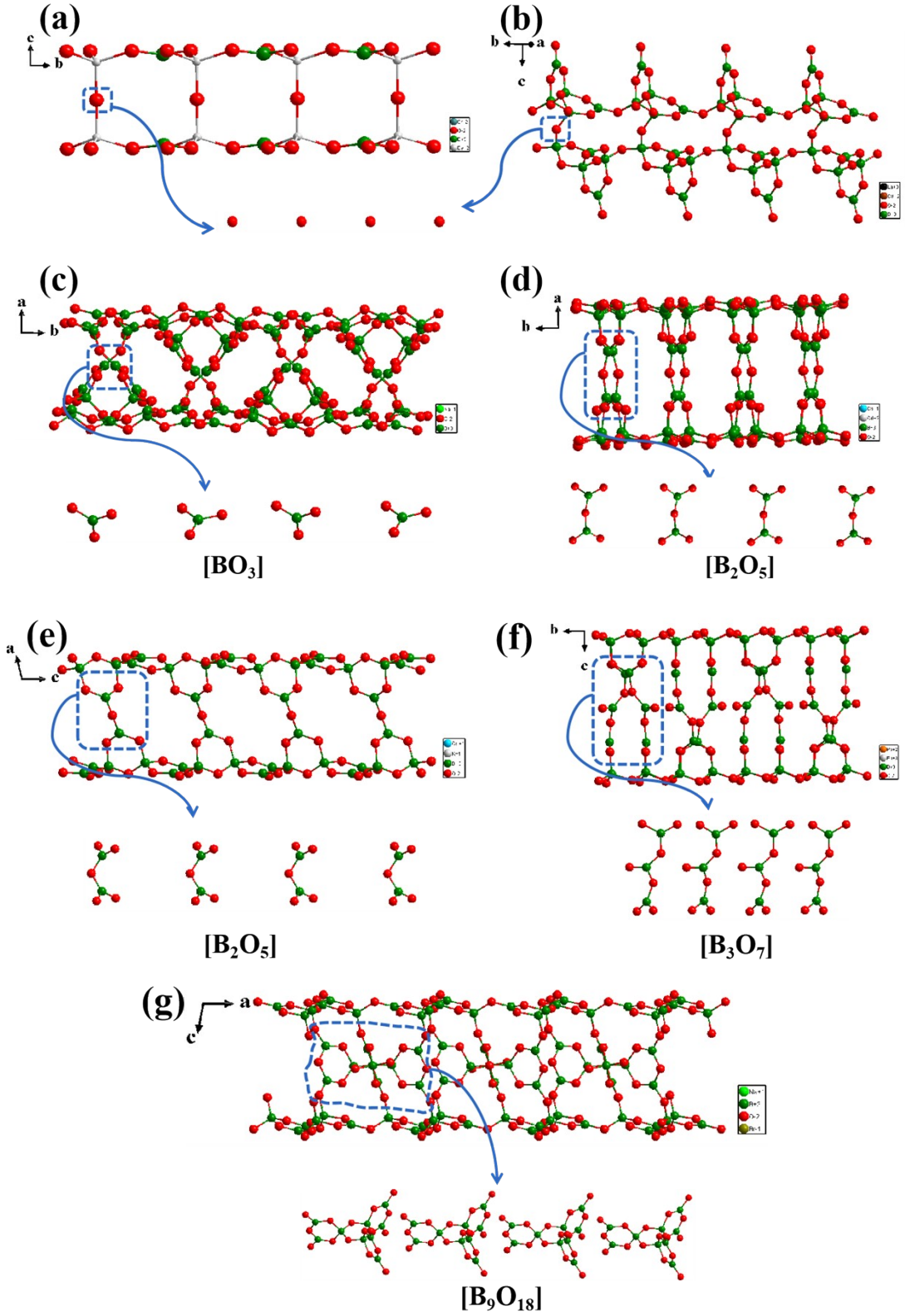


Fig. S3 Different connection motifs between sub layers in layered structures $Sr_2Be_2B_2O_7$ (a), $La_2CaB_{10}O_{19}$ (b), $Na_2B_6O_{10}$ (c), $Cd_3Cs_2B_{16}O_{28}$ (d), $Cs_2K_2B_{10}O_{17}$ (e), $PbEuB_7O_{13}$ (f) and $Na_{11}B_{21}O_{36}Br_2$ (g).

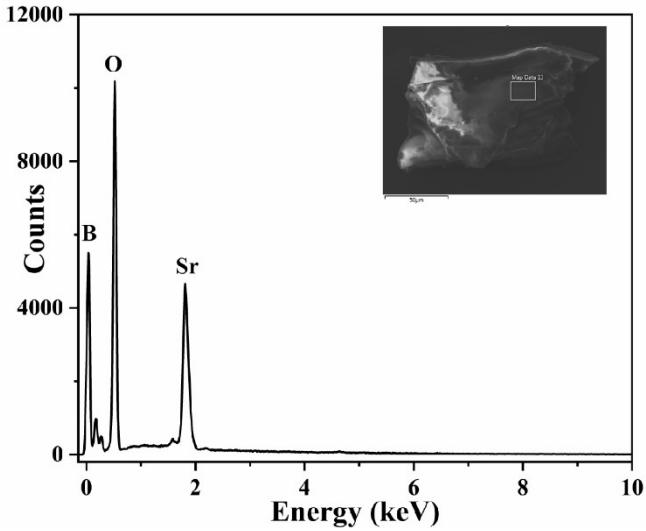


Fig. S4 Energy dispersive X-ray spectroscopy (EDS).

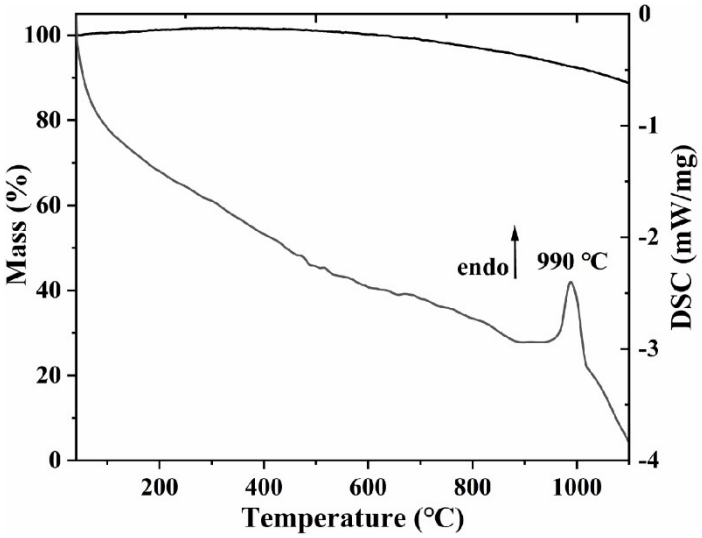


Fig. S5 TG-DSC curves.

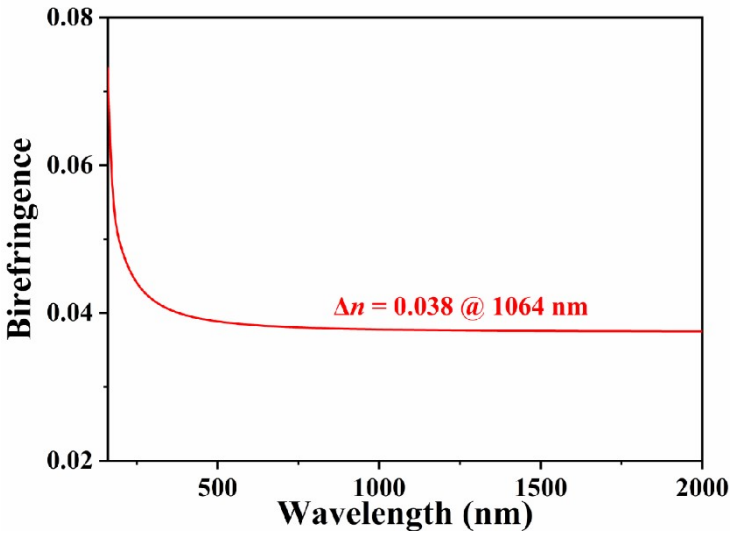


Fig. S6 The calculated birefringence of $Sr_3B_{14}O_{24}$.