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Electronic Supplementary Information:

$Na_2SrB_{16}O_{26}$: A New Borate with Independent Interpenetrating B–O Networks and Deep-Ultraviolet Cutoff Edge

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Table S1. Atomic coordinates (× 10^4), equivalent isotropic displacement parameters (Å^2 × 10^3) and bond valence sum (BVS) calculation for $Na_2SrB_{16}O_{26}$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}[a]	BVS[b]
Sr1	5000	5000	10000	26(1)	2.0
Na1	8831(1)	3960(3)	6829(2)	49(1)	0.9
B1	10607(2)	1845(3)	4544(3)	12(1)	3.0
B2	8913(2)	3935(4)	3908(3)	13(1)	3.0
B3	7325(2)	5890(4)	3833(3)	11(1)	3.0
B4	6185(2)	5943(4)	5600(3)	11(1)	3.0
B5	5011(2)	6450(4)	7216(3)	10(1)	3.0
B6	3610(2)	8902(3)	7533(3)	9(1)	3.1
B7	2080(2)	9794(4)	5509(3)	12(1)	3.0
B8	1837(2)	10518(4)	3147(3)	12(1)	3.0
O1	11123(2)	848(3)	5598(2)	15(1)	1.9
O2	10985(2)	1840(3)	3403(2)	17(1)	1.9
O3	9689(2)	2879(2)	4752(2)	13(1)	2.0
O4	8893(2)	4143(3)	2627(2)	17(1)	2.0
O5	8195(2)	4865(2)	4562(2)	14(1)	2.1
O6	7320(2)	6271(2)	2571(2)	14(1)	1.9
O7	6670(2)	4530(2)	6234(2)	12(1)	2.0
O8	6470(2)	6539(2)	4456(2)	14(1)	2.0
O9	5296(2)	6887(2)	6018(2)	12(1)	2.1
O10	5584(2)	5105(2)	7916(2)	11(1)	2.3
O11	4172(1)	7210(2)	7752(2)	11(1)	2.0
O12	2508(2)	8791(2)	6561(2)	14(1)	2.0
O13	2514(2)	9783(2)	4388(2)	16(1)	1.9

[a]U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

[b]BVS are calculated by using the bond-valence model ($S_i = \exp[(R_o - R_i)/B]$, where R_o is an empirical constant, R_i is the length of bond (in angstroms), and B = 0.37.

Table S2. Selected bond lengths (Å) and angles (°) for $Na_2SrB_{16}O_{26}$.

Sr(1)-O(11)	2.8943(18)	B(2)-O(5)	1.379(3)
Sr(1)-O(11)#1	2.8942(18)	B(3)-O(5)	1.378(3)
Sr(1)-O(9)#2	2.6274(18)	B(3)-O(6)	1.342(3)
Sr(1)-O(9)#3	2.6274(18)	B(3)-O(8)	1.382(3)
Sr(1)-O(8)#3	3.2843(18)	B(4)-O(7)	1.339(3)
Sr(1)-O(8)#2	3.2843(18)	B(4)-O(8)	1.377(3)
Sr(1)-O(10)#1	2.3984(19)	B(4)-O(9)	1.401(3)
Sr(1)-O(10)	2.3984(19)	B(5)-O(9)	1.393(3)
Sr(1)-O(13)#2	2.8137(19)	B(5)-O(10)	1.361(3)
Sr(1)-O(13)#3	2.8137(19)	B(5)-O(11)	1.348(3)
Na(1)-O(7)	2.483(2)	B(6)-O(7)#2	1.467(3)
Na(1)-O(3)	2.688(2)	B(6)-O(10)#2	1.460(3)
Na(1)-O(5)	2.421(2)	B(6)-O(11)	1.460(3)
Na(1)-O(2)#4	2.750(2)	B(6)-O(12)	1.454(3)
Na(1)-O(12)#2	2.503(2)	B(7)-O(1)#7	1.392(3)
Na(1)-O(4)#4	2.538(3)	B(7)-O(12)	1.349(3)
Na(1)-O(4)#5	2.962(3)	B(7)-O(13)	1.360(4)
B(1)-O(1)	1.372(3)	B(8)-O(2)#7	1.481(3)
B(1)-O(2)	1.345(4)	B(8)-O(4)#6	1.487(3)
B(1)-O(3)	1.380(3)	B(8)-O(6)#6	1.465(3)
B(2)-O(3)	1.384(3)	B(8)-O(13)	1.476(3)
B(2)-O(4)	1.336(3)		
O(11)#1-Sr(1)-O(11)	180.00(5)	O(7)-Na(1)-O(4)#4	102.06(9)
O(11)#1-Sr(1)-O(8)#2	58.28(5)	O(7)-Na(1)-O(4)#5	139.94(10)
O(11)-Sr(1)-O(8)#2	121.72(5)	O(3)-Na(1)-O(2)#4	88.21(7)
O(11)#1-Sr(1)-O(8)#3	121.72(5)	O(3)-Na(1)-O(4)#5	81.25(6)
O(11)-Sr(1)-O(8)#3	58.28(5)	O(5)-Na(1)-O(7)	67.60(7)
O(9)#2-Sr(1)-O(11)	102.96(5)	O(5)-Na(1)-O(3)	52.94(6)

O(9)#2-Sr(1)-O(11)#1	77.04(5)	O(5)-Na(1)-O(2)#4	134.32(8)
O(9)#3-Sr(1)-O(11)	77.04(5)	O(5)-Na(1)-O(12)#2	124.03(8)
O(9)#3-Sr(1)-O(11)#1	102.96(5)	O(5)-Na(1)-O(4)#5	96.91(8)
O(9)#3-Sr(1)-O(9)#2	180	O(5)-Na(1)-O(4)#4	125.05(11)
O(9)#3-Sr(1)-O(8)#3	44.86(5)	O(2)#4-Na(1)-O(4)#5	48.76(6)
O(9)#2-Sr(1)-O(8)#3	135.14(5)	O(12)#2-Na(1)-O(3)	154.25(11)
O(9)#3-Sr(1)-O(8)#2	135.14(5)	O(12)#2-Na(1)-O(2)#4	101.46(7)
O(9)#2-Sr(1)-O(8)#2	44.86(5)	O(12)#2-Na(1)-O(4)#4	73.27(7)
O(9)#2-Sr(1)-O(13)#2	94.46(5)	O(12)#2-Na(1)-O(4)#5	122.99(9)
O(9)#3-Sr(1)-O(13)#2	85.54(5)	O(4)#4-Na(1)-O(3)	88.68(9)
O(9)#3-Sr(1)-O(13)#3	94.46(5)	O(4)#4-Na(1)-O(2)#4	68.38(7)
O(9)#2-Sr(1)-O(13)#3	85.54(5)	O(4)#4-Na(1)-O(4)#5	116.35(6)
O(8)#3-Sr(1)-O(8)#2	180	O(1)-B(1)-O(3)	115.0(2)
O(10)-Sr(1)-O(11)#1	129.87(5)	O(2)-B(1)-O(3)	122.6(2)
O(10)#1-Sr(1)-O(11)#1	50.13(5)	O(2)-B(1)-O(1)	122.3(2)
O(10)-Sr(1)-O(11)	50.13(5)	O(5)-B(2)-O(3)	111.9(2)
O(10)#1-Sr(1)-O(11)	129.87(5)	O(4)-B(2)-O(3)	125.3(2)
O(10)-Sr(1)-O(9)#2	72.85(6)	O(4)-B(2)-O(5)	122.6(2)
O(10)#1-Sr(1)-O(9)#3	72.85(6)	O(6)-B(3)-O(8)	121.2(2)
O(10)#1-Sr(1)-O(9)#2	107.15(6)	O(6)-B(3)-O(5)	121.3(2)
O(10)-Sr(1)-O(9)#3	107.15(6)	O(5)-B(3)-O(8)	117.5(2)
O(10)-Sr(1)-O(8)#3	64.22(5)	O(7)-B(4)-O(9)	122.2(2)
O(10)#1-Sr(1)-O(8)#2	64.22(5)	O(7)-B(4)-O(8)	123.3(2)
O(10)-Sr(1)-O(8)#2	115.78(5)	O(8)-B(4)-O(9)	114.4(2)
O(10)#1-Sr(1)-O(8)#3	115.78(5)	O(11)-B(5)-O(9)	125.8(2)
O(10)#1-Sr(1)-O(10)	180	O(11)-B(5)-O(10)	115.2(2)
O(10)-Sr(1)-O(13)#2	75.06(6)	O(10)-B(5)-O(9)	119.0(2)
O(10)#1-Sr(1)-	75.06(6)	O(11)-B(6)-O(7)#8	109.5(2)

O(13)#3			
O(10)#1-Sr(1)-O(13)#2	104.94(6)	O(11)-B(6)-O(10)#8	109.32(19)
O(10)-Sr(1)-O(13)#3	104.94(6)	O(10)#8-B(6)-O(7)#8	109.7(2)
O(13)#3-Sr(1)-O(11)	68.35(5)	O(12)-B(6)-O(11)	110.6(2)
O(13)#2-Sr(1)-O(11)	111.65(5)	O(12)-B(6)-O(7)#8	107.8(2)
O(13)#3-Sr(1)-O(11)#1	111.65(5)	O(12)-B(6)-O(10)#8	109.9(2)
O(13)#2-Sr(1)-O(11)#1	68.35(5)	O(12)-B(7)-O(1)#10	116.5(2)
O(13)#3-Sr(1)-O(8)#3	116.85(5)	O(12)-B(7)-O(13)	123.6(2)
O(13)#2-Sr(1)-O(8)#3	63.15(5)	O(13)-B(7)-O(1)#10	119.9(2)
O(13)#2-Sr(1)-O(8)#2	116.85(5)	O(6)#11-B(8)-O(2)#10	110.6(2)
O(13)#3-Sr(1)-O(8)#2	63.15(5)	O(6)#11-B(8)-O(4)#11	111.8(2)
O(13)#3-Sr(1)-O(13)#2	180.00(8)	O(6)#11-B(8)-O(13)	108.1(2)
O(7)-Na(1)-O(3)	111.93(8)	O(2)#10-B(8)-O(4)#11	105.7(2)
O(7)-Na(1)-O(2)#4	157.99(9)	O(13)-B(8)-O(2)#10	111.2(2)
O(7)-Na(1)-O(12)#2	56.53(7)	O(13)-B(8)-O(4)#11	109.5(2)

Symmetry transformations used to generate equivalent atoms:

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

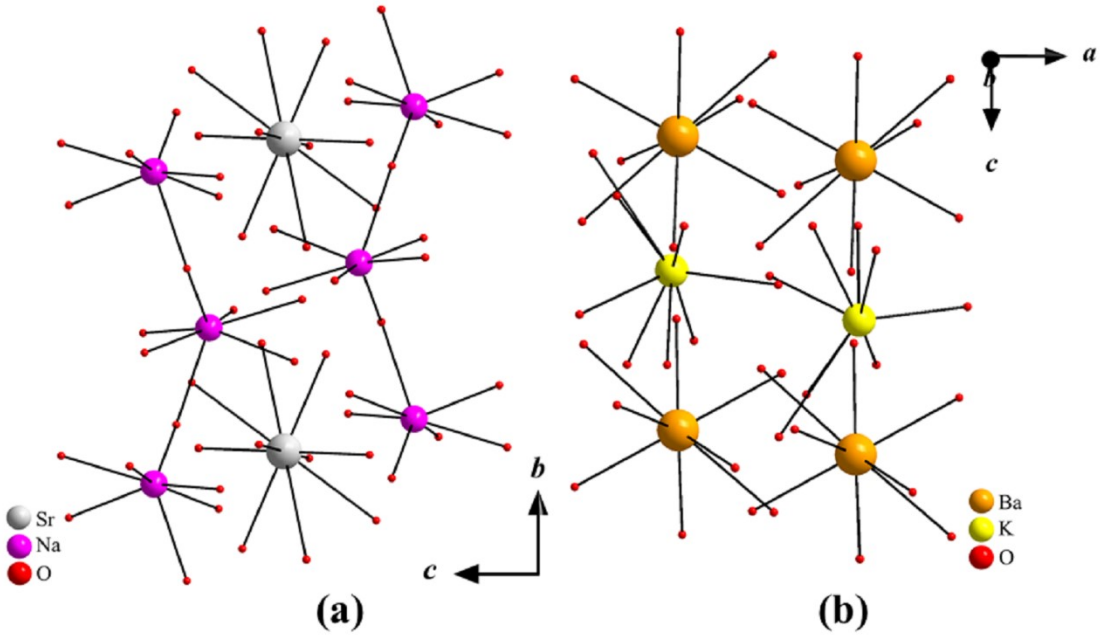

Figure S1. (a) The Na−O chains and isolated [SrO_{10}] groups in $Na_2SrB_{16}O_{26}$; (b)The isolated [KO_8] and [BaO_8] groups in $K_2BaB_{16}O_{26}$.

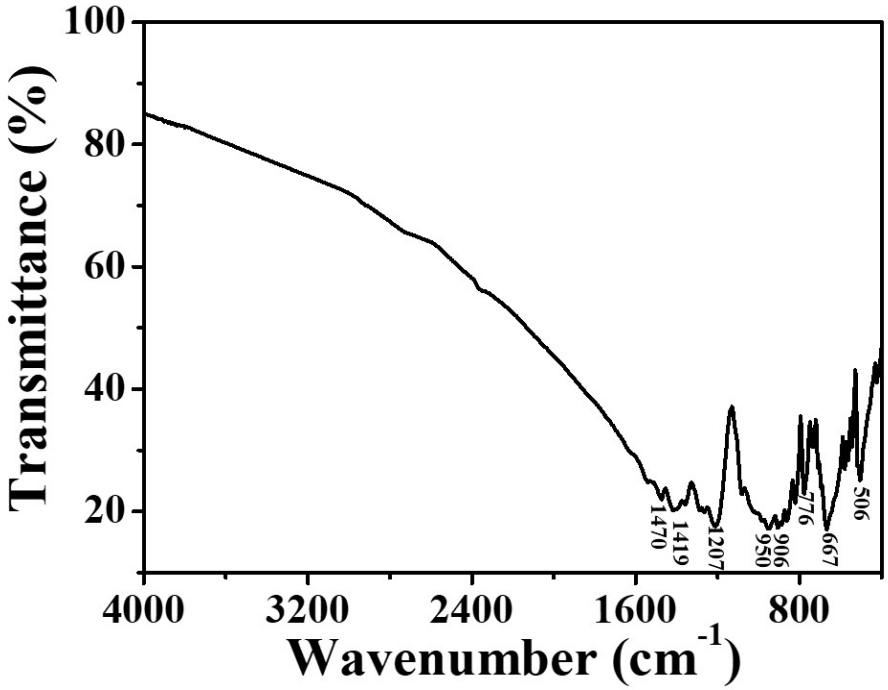

Figure S2. IR spectrum.

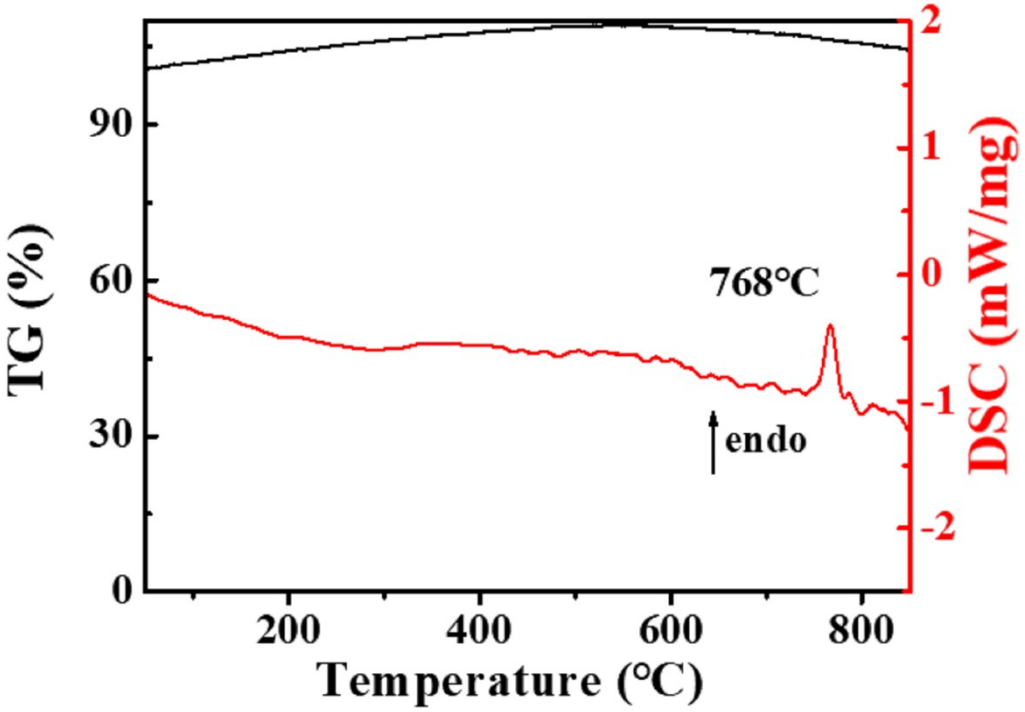

Figure S3. TG-DSC curves.

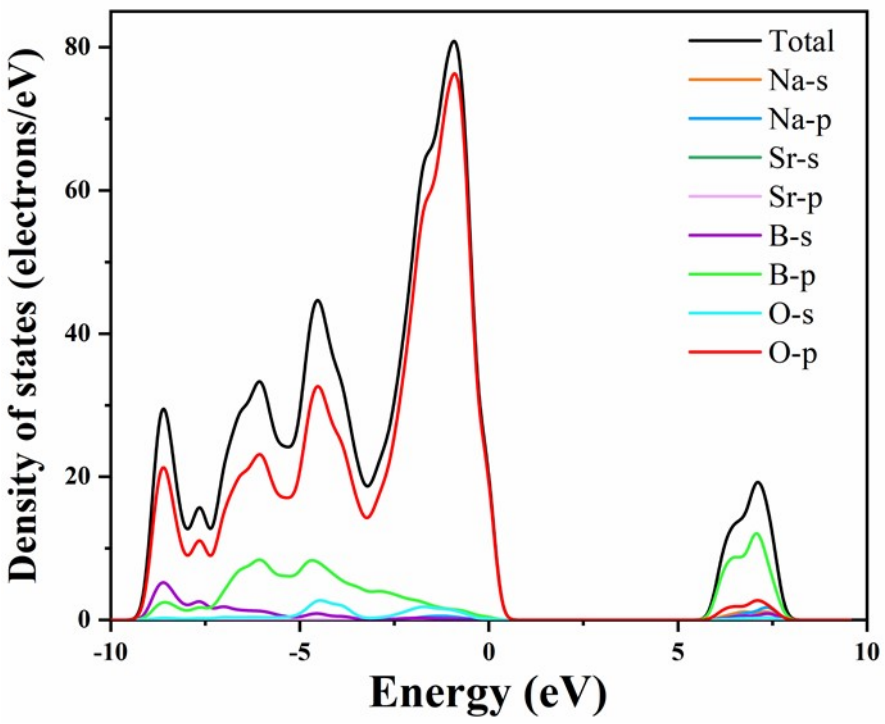

Figure S4. Density of states (DOS).