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Supporting Information

$Ba_2B_{10}O_{17}$: A New Centrosymmetric Alkaline-Earth Metal Borate with Deep-UV Cut-Off Edge

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Table S1 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Ba_2B_{10}O_{17}$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ba(1)	2483(1)	9802(1)	2217(1)	10(1)
Ba(2)	2731(1)	5234(1)	2974(1)	12(1)
B(1)	2228(6)	1973(5)	-1299(4)	8(1)
B(2)	130(6)	2669(5)	4827(4)	8(1)
B(3)	-2941(6)	7041(5)	3825(5)	10(1)
B(4)	4818(6)	2323(5)	267(4)	8(1)
B(5)	-1457(6)	2433(5)	-243(4)	8(1)
B(6)	2622(6)	4957(5)	-288(5)	11(1)
B(7)	2413(7)	50(5)	5447(5)	11(1)
B(8)	-1965(6)	3872(5)	2813(4)	8(1)
B(9)	3582(7)	7468(5)	5172(5)	10(1)
B(10)	-2561(6)	1106(5)	1989(4)	10(1)
O(1)	3767(4)	3764(3)	544(3)	12(1)
O(2)	1529(4)	6039(3)	347(3)	12(1)
O(3)	3373(4)	7697(3)	710(3)	10(1)
O(4)	6565(4)	3162(3)	3349(3)	10(1)
O(5)	-207(4)	3664(3)	3446(3)	11(1)
O(6)	3770(4)	8963(3)	4899(3)	11(1)
O(7)	5475(4)	1350(3)	1623(3)	9(1)
O(8)	1846(4)	7442(3)	4461(3)	12(1)
O(9)	1543(4)	1298(3)	4565(3)	13(1)
O(10)	6570(4)	7825(3)	2529(3)	12(1)
O(11)	-1798(4)	135(3)	3183(3)	11(1)
O(12)	-218(4)	8061(3)	1269(3)	10(1)
O(13)	-1058(4)	1611(3)	1153(3)	11(1)
O(14)	7480(4)	4976(3)	1664(3)	13(1)
O(15)	3265(4)	1692(3)	-133(3)	12(1)
O(16)	-1026(4)	6653(3)	4311(3)	15(1)
O(17)	4483(4)	3441(3)	5372(3)	15(1)

Table S2 Bond lengths (Å) and angles (°) for $Ba_2B_{10}O_{17}$.

Ba(1)-O(10)	2.879(3)	O(13)-Ba(1)-O(3)	102.26(8)
Ba(1)-O(11)	2.871(2)	O(13)-Ba(1)-O(15)	68.05(8)
Ba(1)-O(12)	3.174(3)	O(3)-Ba(1)-O(15)	88.48(8)
Ba(1)-O(13)	2.697(3)	O(13)-Ba(1)-O(6)	131.29(8)
Ba(1)-O(15)	2.748(3)	O(3)-Ba(1)-O(6)	116.66(8)
Ba(1)-O(3)	2.728(3)	O(15)-Ba(1)-O(6)	136.50(8)
Ba(1)-O(6)	2.784(3)	O(13)-Ba(1)-O(7)	106.41(8)
Ba(1)-O(7)	2.790(2)	O(3)-Ba(1)-O(7)	110.41(7)
Ba(1)-O(8)	2.934(3)	O(15)-Ba(1)-O(7)	49.89(8)
Ba(1)-O(9)	2.963(3)	O(6)-Ba(1)-O(7)	87.07(7)
Ba(2)-O(1)	3.019(3)	O(13)-Ba(1)-O(11)	48.82(8)
Ba(2)-O(12)	3.175(3)	O(3)-Ba(1)-O(11)	105.34(7)
Ba(2)-O(14)	3.262(3)	O(15)-Ba(1)-O(11)	116.81(8)
Ba(2)-O(16)	2.853(3)	O(6)-Ba(1)-O(11)	91.41(7)
Ba(2)-O(16)#2	3.215(3)	O(7)-Ba(1)-O(11)	140.62(8)
Ba(2)-O(17)	2.794(3)	O(13)-Ba(1)-O(10)	163.33(8)
Ba(2)-O(2)	2.714(3)	O(3)-Ba(1)-O(10)	65.08(8)
Ba(2)-O(3)	3.015(3)	O(15)-Ba(1)-O(10)	99.65(8)
Ba(2)-O(4)	2.794(3)	O(6)-Ba(1)-O(10)	65.37(7)
Ba(2)-O(5)	2.778(2)	O(7)-Ba(1)-O(10)	70.54(8)
Ba(2)-O(8)	2.800(3)	O(11)-Ba(1)-O(10)	142.47(8)
B(1)-O(10)#9	1.396(5)	O(13)-Ba(1)-O(8)	114.35(7)
B(1)-O(12)#1	1.356(5)	O(3)-Ba(1)-O(8)	82.60(8)
B(1)-O(15)	1.362(5)	O(15)-Ba(1)-O(8)	171.06(8)
B(2)-O(16)#8	1.473(5)	O(6)-Ba(1)-O(8)	49.07(7)
B(2)-O(5)#7	1.501(5)	O(7)-Ba(1)-O(8)	133.37(7)
B(2)-O(8)#8	1.450(5)	O(11)-Ba(1)-O(8)	66.54(8)
B(2)-O(9)	1.471(5)	O(10)-Ba(1)-O(8)	76.10(7)
B(3)-O(10)#10	1.373(5)	O(13)-Ba(1)-O(9)	87.70(8)
B(3)O-(16)	1.348(5)	O(3)-Ba(1)-O(9)	162.02(8)
B(3)-O(17)#2	1.362(5)	O(15)-Ba(1)-O(9)	109.23(8)
B(4)-O(1)	1.468(5)	O(6)-Ba(1)-O(9)	47.80(8)
B(4)-O(15)#6	1.489(5)	O(7)-Ba(1)-O(9)	80.37(7)
B(4)-O(3)#3	1.464(4)	O(11)-Ba(1)-O(9)	69.95(7)
B(4)-O(7)#6	1.504(5)	O(10)-Ba(1)-O(9)	107.50(8)
B(5)-O(2) #1	1.468 (5)	O(8)-Ba(1)-O(9)	79.65(8)
B(5)-O(12)#1	1.482(4)	O(13)-Ba(1)-O(12)	69.32(8)
B(5)-O(12)	1.475 (5)	O(3)-Ba(1)-O(12)	46.19(7)
B(5)-O(3) #1	1.458(5)	O(15)-Ba(1)-O(12)	104.58(7)
B(6)-O(1)	1.363(5)	O(6)-Ba(1)-O(12)	118.54(7)
B(6)-O(14)#3	1.371(5)	O(7)-Ba(1)-O(12)	150.16(7)

B(6)-O(2)	1.352(5)	O(11)-Ba(1)-O(12)	59.36(7)
B(7)-O(11)#8	1.370(5)	O(10)-Ba(1)-O(12)	104.77(7)
B(7)-O(6)	1.367(5)	O(8)-Ba(1)-O(12)	69.48(7)
B(7)-O(9)	1.361(6)	O(9)-Ba(1)-O(12)	127.64(7)
B(8)-O(14)#10	1.395(5)	O(2)-Ba(2)-O(5)	85.37(8)
B(8)-O(4)#10	1.361(5)	O(2)-Ba(2)-O(17)	159.02(9)
B(8)-O(5)	1.347(5)	O(5)-Ba(2)-O(17)	86.28(8)
B(9)-O(17)#5	1.475(5)	O(2)-Ba(2)-O(4)	114.75(8)
B(9)-O(4)#5	1.472(5)	O(5)-Ba(2)-O(4)	105.05(8)
B(9)-O(6)	1.477(5)	O(17)-Ba(2)-O(4)	49.56(7)
B(9)-O(8)	1.444(5)	O(2)-Ba(2)-O(8)	115.95(8)
B(10)#4-O(7)	1.349(5)	O(5)-Ba(2)-O(8)	113.83(8)
B(10)-O(11)	1.396(5)	O(17)-Ba(2)-O(8)	85.03(8)
B(10)-O(13)	1.365(5)	O(4)-Ba(2)-O(8)	116.98(8)
O(8)-B(9)-O(4)#5	112.6(3)	O(2)-Ba(2)-O(16)	98.92(8)
O(8)-B(9)-O(17)#5	109.2(3)	O(5)-Ba(2)-O(16)	67.82(8)
O(4)#5-B(9)-O(17)#5	105.2(3)	O(17)-Ba(2)-O(16)	95.68(8)
O(8)-B(9)-O(6)	109.0(3)	O(4)-Ba(2)-O(16)	145.23(8)
O(4)#5-B(9)-O(6)	112.7(3)	O(8)-Ba(2)-O(16)	48.20(7)
O(17)#5-B(9)-O(6)	108.0(3)	O(2)-Ba(2)-O(3)	49.77(8)
O(7)#10-B(10)-O(13)	123.7(4)	O(5)-Ba(2)-O(3)	132.37(7)
O(7)#10-B(10)-O(11)	122.4(3)	O(17)-Ba(2)-O(3)	141.33(7)
O(13)-B(10)-O(11)	113.3(3)	O(4)-Ba(2)-O(3)	107.84(7)
O(13)-B(5)-O(12)#1	113.1(3)	O(8)-Ba(2)-O(3)	79.97(8)
O(3)#1-B(5)-O(12)#1	105.7(3)	O(16)-Ba(2)-O(3)	100.25(8)
O(2)#1-B(5)-O(12)#1	104.2(3)	O(2)-Ba(2)-O(1)	46.85(8)
O(2)-B(6)-O(1)	115.4(4)	O(5)-Ba(2)-O(1)	79.38(7)
O(2)-B(6)-O(14)#3	122.6(4)	O(17)-Ba(2)-O(1)	112.58(8)
O(1)-B(6)-O(14)#3	121.9(4)	O(4)-Ba(2)-O(1)	71.60(7)
O(9)-B(7)-O(6)	117.7(4)	O(8)-Ba(2)-O(1)	159.32(8)
O(9)-B(7)-O(11)#8	120.2(4)	O(16)-Ba(2)-O(1)	134.96(7)
O(6)-B(7)-O(11)#8	121.8(4)	O(3)-Ba(2)-O(1)	79.43(7)
O(5)-B(8)-O(4)#10	122.5(4)	O(2)-Ba(2)-O(12)	45.88(8)
O(5)-B(8)-O(14)#10	121.4(4)	O(5)-Ba(2)-O(12)	94.78(7)
O(4)#10-B(8)-O(14)#10	115.5(3)	O(17)-Ba(2)-O(12)	154.37(7)
O(3)#3-B(4)-O(15)#6	113.5(3)	O(4)-Ba(2)-O(12)	151.51(7)
O(1)-B(4)-O(15)#6	109.5(3)	O(8)-Ba(2)-O(12)	71.08(7)
O(3)#3-B(4)-O(7)#6	110.1(3)	O(16)-Ba(2)-O(12)	61.58(7)
O(1)-B(4)-O(7)#6	107.0(3)	O(3)-Ba(2)-O(12)	44.56(6)
O(15)#6-B(4)-O(7)#6	102.6(3)	O(1)-Ba(2)-O(12)	92.72(7)
O(13)-B(5)-O(3)#1	111.5(3)	B(5)#1-Ba(2)-O(12)	27.01(8)
O(13)-B(5)-O(2)#1	111.0(3)	O(2)-Ba(2)-O(16)#2	131.82(7)
O(3)#1-B(5)-O(2)#1	111.0(3)	O(5)-Ba(2)-O(16)#2	46.63(7)

O(17)-Ba(2)-O(16)#2	44.95(7)	O(1)-Ba(2)-O(14)	66.42(7)
O(4)-Ba(2)-O(16)#2	86.61(7)	O(12)-Ba(2)-O(14)	107.77(7)
O(16)#2-Ba(2)-O(14)	130.07(7)	O(8)-Ba(2)-O(16)#2	86.28(7)
O(12)#1-B(1)-O(15)	122.4(3)	O(16)-Ba(2)-O(16)#2	63.43(10)
O(12)#1-B(1)-O(10)#9	122.1(4)	O(3)-Ba(2)-O(16)#2	163.42(7)
O(15)-B(1)-O(10)#9	115.3(3)	O(1)-Ba(2)-O(16)#2	113.70(7)
O(8)#8-B(2)-O(9)	115.0(3)	O(12)-Ba(2)-O(16)#2	121.80(7)
O(8)#8-B(2)-O(16)#8	104.3(3)	O(2)-Ba(2)-O(14)	86.76(7)
O(9)-B(2)-O(16)#8	112.8(3)	O(5)-Ba(2)-O(14)	139.29(8)
O(8)#8-B(2)-O(5)#7	110.6(3)	O(17)-Ba(2)-O(14)	87.08(7)
O(9)-B(2)-O(5)#7	106.0(3)	O(4)-Ba(2)-O(14)	44.45(7)
O(16)#8-B(2)-O(5)#7	108.0(3)	O(8)-Ba(2)-O(14)	105.51(7)
O(16)-B(3)-O(17)#2	118.6(4)	O(16)-Ba(2)-O(14)	152.87(8)
O(16)-B(3)-O(10)#10	124.4(4)	O(3)-Ba(2)-O(14)	63.44(7)
O(17)#2-B(3)-O(10)#10	116.9(3)	O(3)#3-B(4)-O(1)	113.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z	#2 -x,-y+1,-z+1	#3 -x+1,-y+1,-z
#4 x+1,y,z	#5 -x+1,-y+1,-z+1	#6 x,y-1,z
#7 x,y+1,z	#8 -x,-y+2,-z+1	#9 -x+1,-y+2,-z
#10 x-1,y,z		

Table S3 Bond valence analysis of $Ba_2B_{10}O_{17}$. [a,b]

O(8)	O(9)	O(10)	O(11)	O(12)	O(13)	O(14)	O(15)	O(16)	O(17)	Σcation
0.173	0.16	0.201	0.205	0.09	0.328		0.286			2.261
0.249				0.09		0.071		0.215 /0.081		2.066
		0.935		1.041			1.025			3.001
0.808	0.763							0.759		3.034
		0.995						1.064	1.025	3.084
							0.727			2.972
				0.741	0.79					3.056
						1				3.075
	1.027		1.003							3.041
						0.937				3.031
0.821									0.755	3.088
					0.935			1.016		3.012
2.051	1.95	2.131	2.143	1.962	2.134	2.008	2.038	2.119	2.033	

Atom	O(1)	O(2)	O(3)	O(4)	O(5)	O(6)	O(7)
Ba(1)			0.302			0.26	0.255
Ba(2)	0.138	0.314	0.139	0.253	0.264		
B(1)							
B(2)					0.704		
B(3)							
B(4)	0.769		0.778				0.698
B(5)		0.755	0.769				
B(6)	1.022	1.053					
B(7)						1.011	
B(8)				1.027	1.067		
B(9)				0.761		0.751	
B(10)							1.061
Σanions	1.929	2.122	1.988	2.041	2.035	2.022	2.014

a Bond valences calculated with the program Bond Valence Calculator Version 2.00, Hormillosa, C., Healy, S., Stephen, T. McMaster University (1993).

b Valence sums calculated with the formula: $Si = \exp[(R_0-R_i)/B]$, where S_i = valence of bond "i" and B = 0.37. Superscripts indicate the number of equivalent bonds for anions.

Table S4 (a) State energies (eV) of the highest valence band (H-VB) and the lowest conduction band (L-CB) at same k-points of $Ba_2B_{10}O_{17}$. (b) The calculated lattice constants (*a*, *b* and *c*) and angles (α, β and γ) between experimental and theoretical results for $Ba_2B_{10}O_{17}$.

(a)

Compound	K-piont	H-VB (eV)	L-CB (eV)
$Ba_2B_{10}O_{17}$	G (0.000, 0.000, 0.000)	0	6.01063
	F (0.000, 0.500, 0.000)	-0.03226	6.02353
	Q (0.000,0.500, 0.500)	0.0119	5.96668
	Z (0.000,0.000, 0.500)	-0.00808	5.98812
	G (0.000,0.000, 0.000)	0	6.01063

(b)

Lattice parameters	Experimental Value	Calculated Value
a (Å)	6.7128(3)	6.7128(0)
b (Å)	9.8698(4)	9.8698(0)
c (Å)	9.9998(4)	9.9998(0)
α (°)	76.860(3)	76.860(0)
β (°)	83.200(3)	83.200(0)
γ (°)	73.332(3)	73.332(0)
Volume ($Å^3$)	617.07(4)	617.07(0)

Table S5 The calculated bond lengths in comparison with experimental data, bond charge and bond order.

bond type	experiment bond length (Å)	calculation bond length (Å)	bond charge (e)	bond order (e)
Ba(1)-O(10)	2.879(3)	2.8787(3)	1.52	0.02
Ba(1)-O(11)	2.871(2)	2.8713(9)	1.52	-0.01
Ba(1)-O(12)	3.174(3)	3.1744(1)	1.52	0.02
Ba(1)-O(13)	2.697(3)	2.6964(4)	1.52	0.05
Ba(1)-O(15)	2.748(3)	2.7484(4)	1.52	0.04
Ba(1)-O(3)	2.728(3)	2.7286(4)	1.52	0.05
Ba(1)-O(6)	2.784(3)	2.7842(0)	1.52	0.00
Ba(1)-O(7)	2.790(2)	2.7900(6)	1.52	0.06
Ba(1)-O(8)	2.934(3)	2.9346(3)	1.52	0.04
Ba(1)-O(9)	2.963(3)	2.9629(5)	1.52	0.03
Ba(2)-O(1)	3.019(3)	3.0189(2)	1.56	0.03
Ba(2)-O(12)	3.175(3)	3.1749(5)	1.56	0.00
Ba(2)-O(14)	3.262(3)	3.2617(9)	1.56	-0.03
Ba(2)-O(16)	2.853(3)	2.8528(4)	1.56	0.03
Ba(2)-O(16)#2	3.215(3)	2.8528(4)	1.56	0.03
Ba(2)-O(17)	2.794(3)	2.7945(6)	1.56	0.02
Ba(2)-O(2)	2.714(3)	2.7142(6)	1.56	0.00
Ba(2)-O(3)	3.015(3)	3.0148(0)	1.56	0.03
Ba(2)-O(4)	2.794(3)	2.7938(0)	1.56	0.02
Ba(2)-O(5)	2.778(2)	2.7771(6)	1.56	0.06
Ba(2)-O(8)	2.800(3)	2.7996(4)	1.56	0.03
B(1)-O(10)#9	1.396(5)	1.3962(1)	1.02	0.70
B(1)-O(12)#1	1.356(5)	1.3559(1)	1.02	0.82
B(1)-O(15)	1.362(5)	1.3621(4)	1.02	0.81
B(2)-O(16)#8	1.473(5)	1.4725(8)	0.94	0.61
B(2)-O(5)#7	1.501(5)	1.5008(7)	0.94	0.57
B(2)-O(8)#8	1.450(5)	1.4500(5)	0.94	0.68
B(2)-O(9)	1.471(5)	1.4715(3)	0.94	0.62
B(3)-O(10)#10	1.373(5)	1.3730(1)	1.02	0.74
B(3)O-(16)	1.348(5)	1.3476(9)	1.02	0.82
B(3)-O(17)#2	1.362(5)	1.3618(1)	1.02	0.78
B(4)-O(1)	1.468(5)	1.4678(1)	0.95	0.61
B(4)-O(15)#6	1.489(5)	1.4896(7)	0.95	0.59
B(4)-O(3)#3	1.464(4)	1.4641(0)	0.95	0.67
B(4)-O(7)#6	1.504(5)	1.5040(0)	0.95	0.57
B(5)-O(12)#1	1.482(4)	1.4813(5)	0.92	0.59
B(5)-O(13)	1.458(5)	1.4586(4)	0.92	0.60
B(5)-O(2) #1	1.468 (5)	1.4749(9)	0.92	0.62
B(5)-O(3) #1	1.458(5)	1.4672(9)	0.92	0.67
B(6)-O(1)	1.363(5)	1.3624(5)	1.02	0.80
B(6)-O(14)#3	1.371(5)	1.3713(9)	1.02	0.74

B(6)-O(2)	1.352(5)	1.3529(5)	1.02	0.80
B(7)-O(11)#8	1.370(5)	1.3697(4)	1.01	0.75
B(7)-O(6)	1.367(5)	1.3673(2)	1.01	0.79
B(7)-O(9)	1.361(6)	1.3607(2)	1.01	0.81
B(8)-O(14)#10	1.395(5)	1.3948(2)	1.01	0.72
B(8)-O(4)#10	1.361(5)	1.3611(5)	1.01	0.81
B(8)-O(5)	1.347(5)	1.3469(6)	1.01	0.82
B(9)-O(17)#5	1.475(5)	1.4744(8)	0.92	0.59
B(9)-O(4)#5	1.472(5)	1.4718(2)	0.92	0.60
B(9)-O(6)	1.477(5)	1.4775(6)	0.92	0.61
B(9)-O(8)	1.444(5)	1.4442(4)	0.92	0.68
B(10) -O(7)	1.349(5)	1.3498(8)	1.00	0.83
B(10)-O(11)	1.396(5)	1.3961(9)	1.00	0.71
B(10)-O(13)	1.365(5)	1.3654(8)	1.00	0.80

Figure S1 Photograph of the $Ba_2B_{10}O_{17}$ crystal. (The minimum scale of the ruler is one millimeter.)

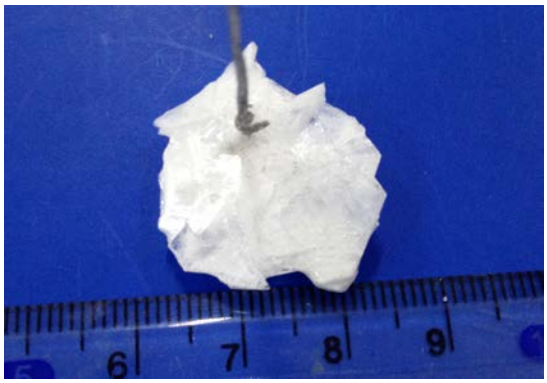


Figure S2 Calculated and measured (after melting and before melting) powder X-ray diffraction patterns for $Ba_2B_{10}O_{17}$.

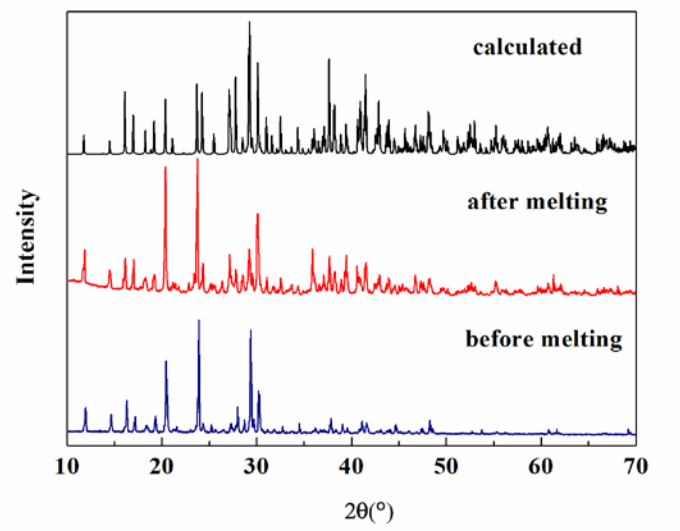


Figure S3 Photograph of the $Ba_2B_{10}O_{17}$ crystal. (The minimum scale of the ruler is one millimeter.)

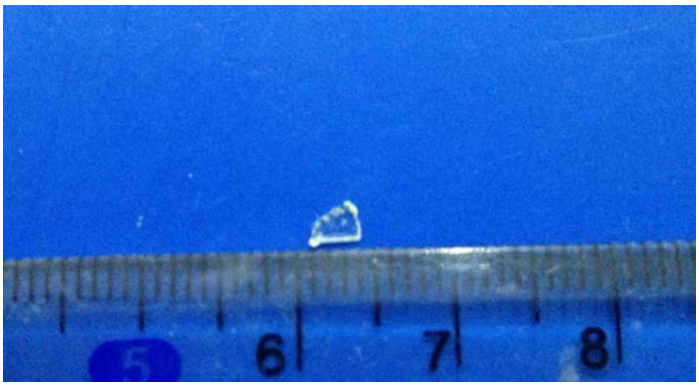


Figure S4 Unit cell of $Ba_2B_{10}O_{17}$.

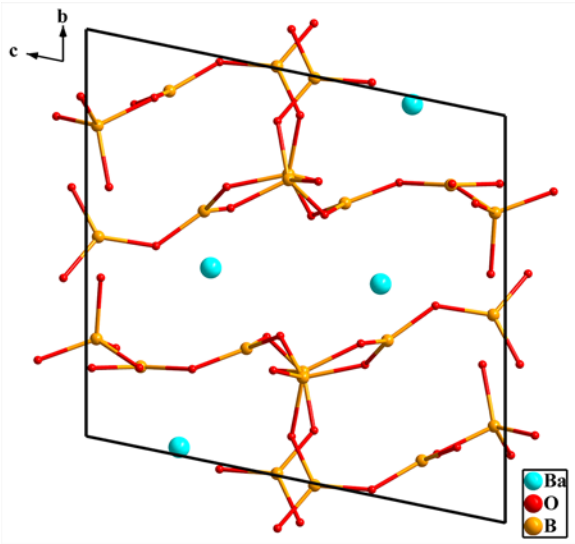


Figure S5 (a) $[Ba(1)O_{10}]$ polyhedra. (b) $[Ba(2)_2O_{20}]$ dimers. (c) Perspective views of $Ba_2B_{10}O_{17}$ along *a*-axis.

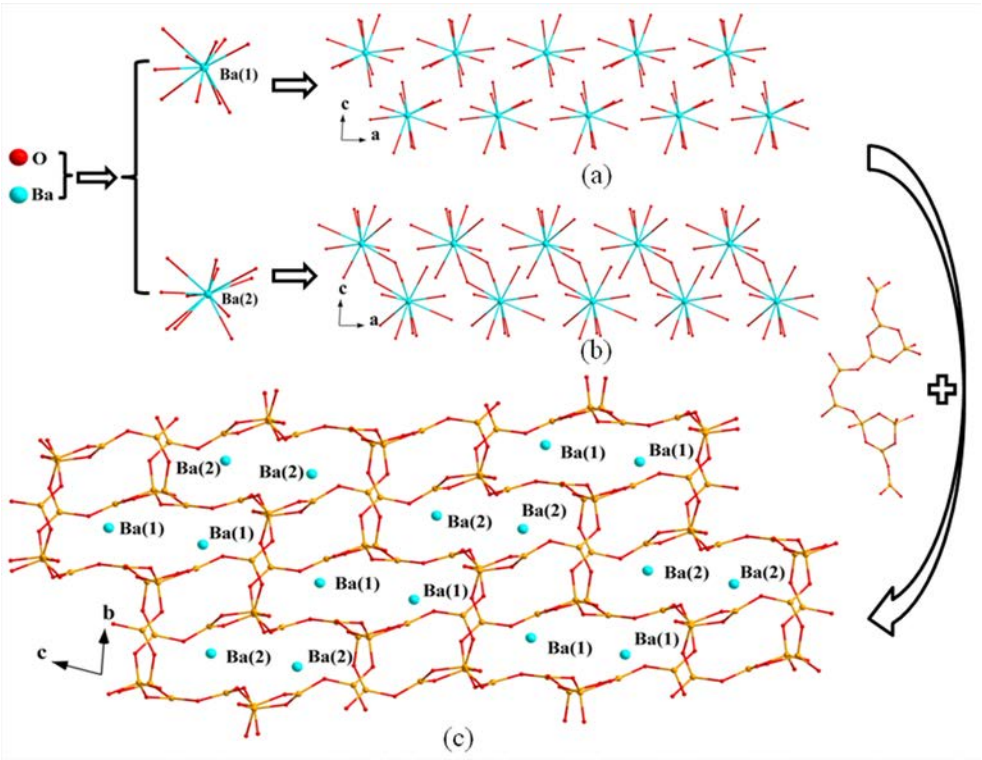


Figure S6 (a) Interconnection between A-tunnel and B-tunnel. (b) The 3D network structure of B-O group in $Ba_2B_{10}O_{17}$. (c) The overall view of $Ba_2B_{10}O_{17}$ seen along the *a*-axis.

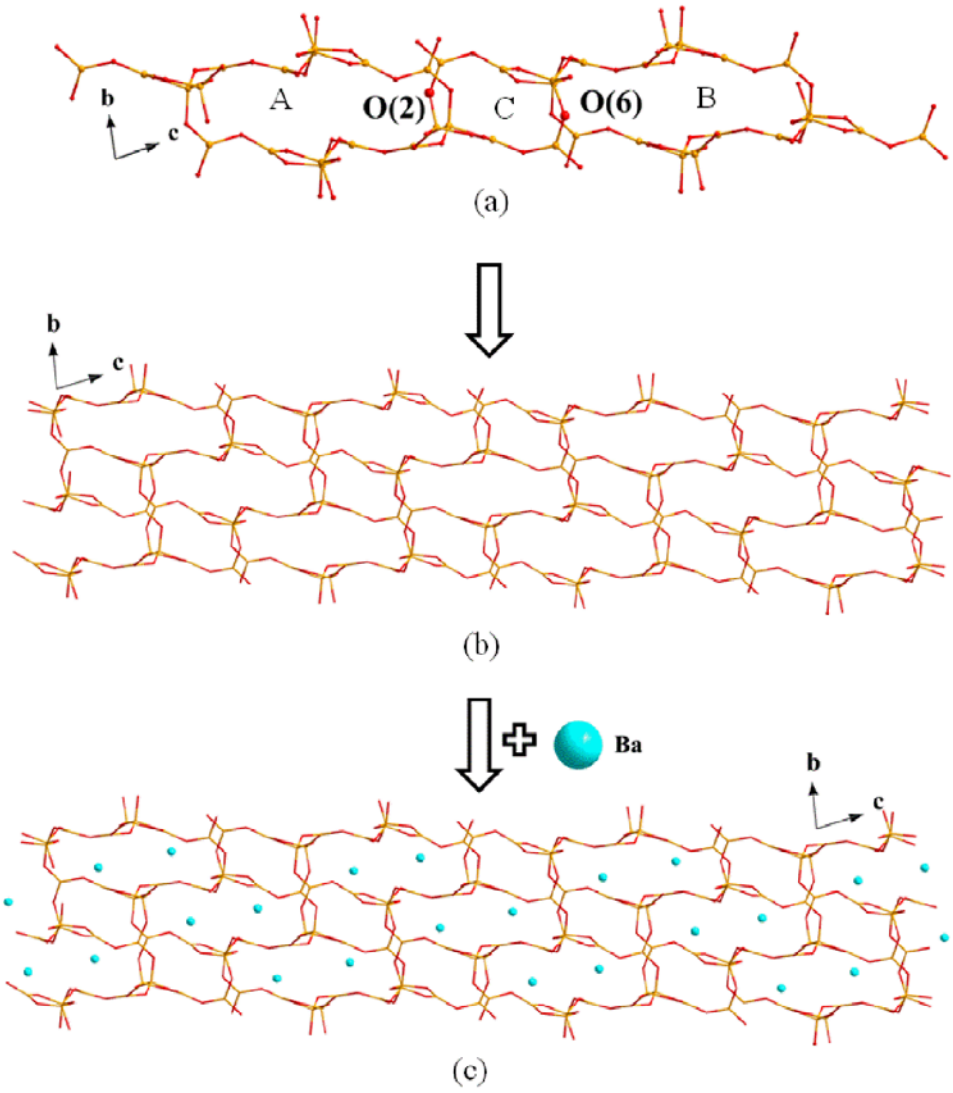


Figure S7 The unit cells of (a) $Cs_2K_2B_{10}O_{17}$, (b) $Na_2Cs_2B_{10}O_{17}$ and (c) $Na_2Tl_2B_{10}O_{17}$.

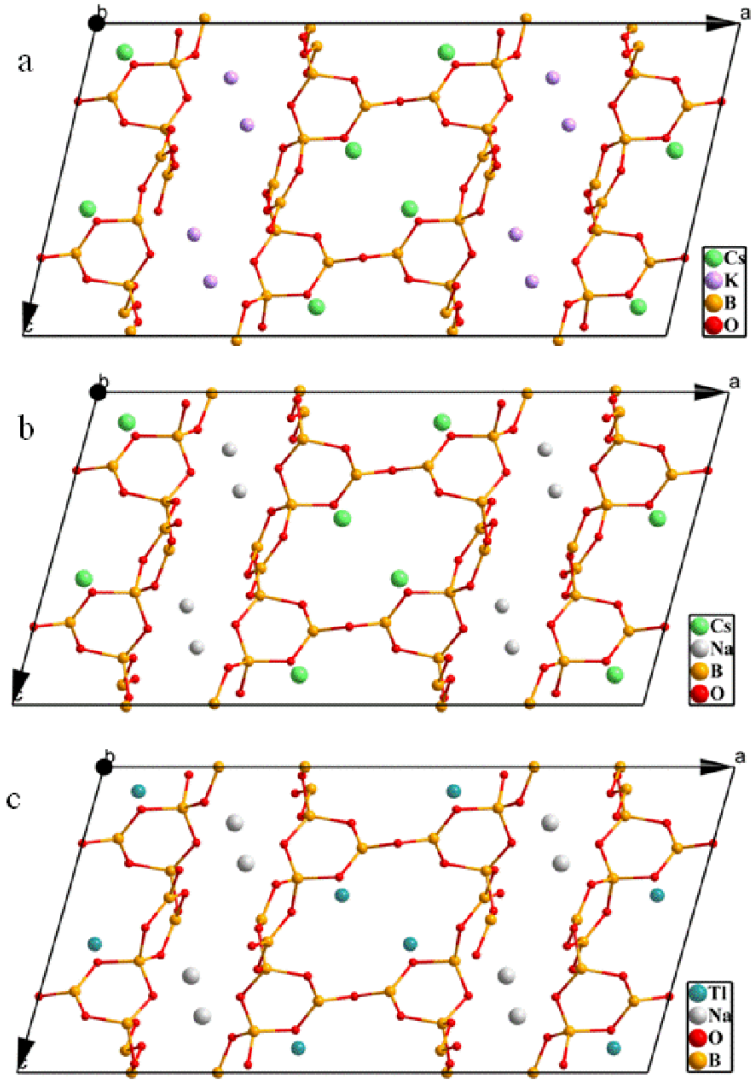


Figure S8 Infrared spectroscopy of $Ba_2B_{10}O_{17}$.

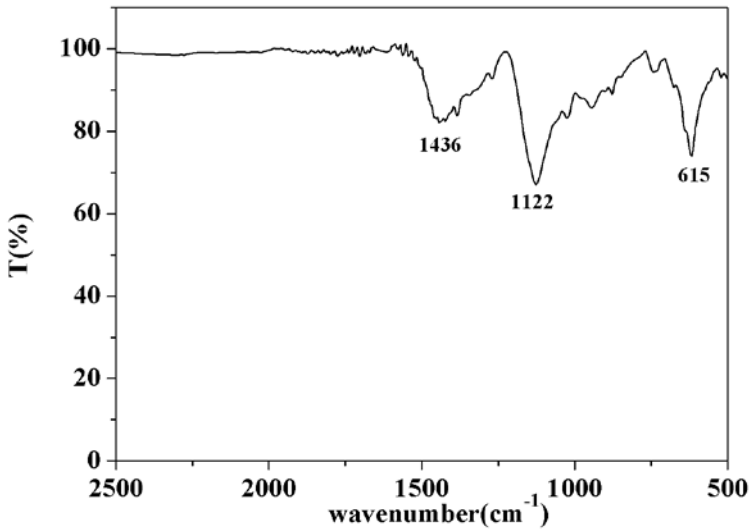


Figure S9 Transmittance spectroscopy of $Ba_2B_{10}O_{17}$.

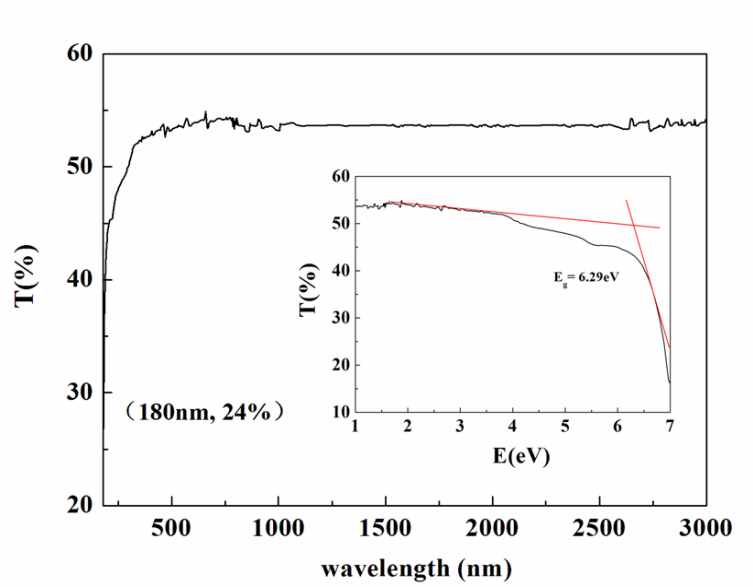


Figure S10 The TG-DSC curves for $Ba_2B_{10}O_{17}$.

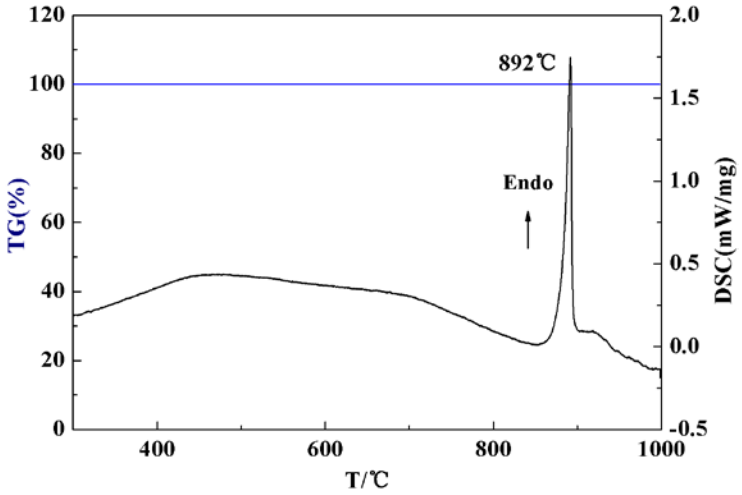


Figure S11 Calculated band structure of $Ba_2B_{10}O_{17}$.

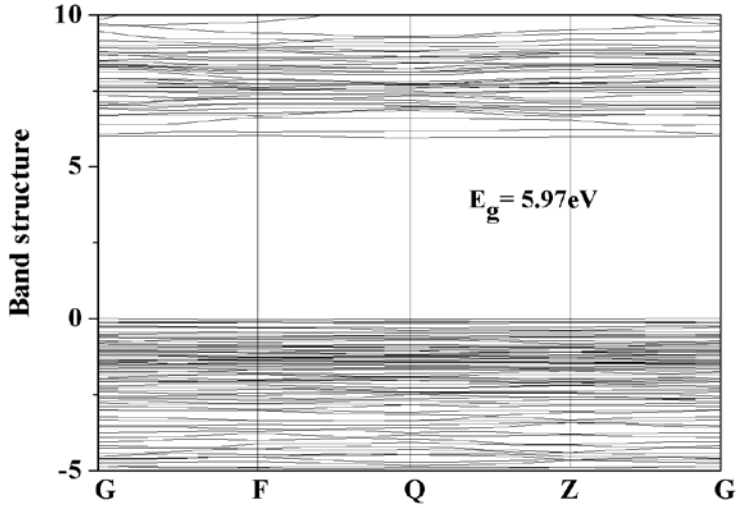
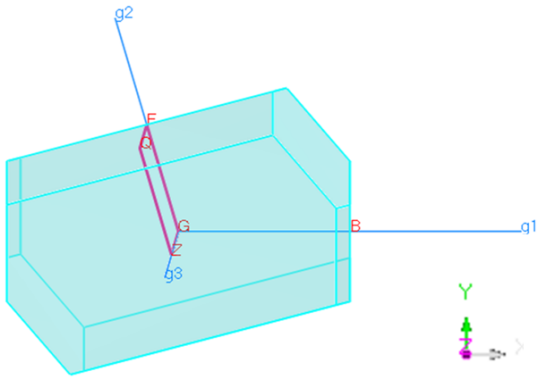


Figure S12 Brillouin zone of $Ba_2B_{10}O_{17}$.



G (0.000, 0.000, 0.000) F (0.000, 0.500, 0.000)

Q (0.000,0.500, 0.500) Z (0.000,0.000, 0.500)

G (0.000,0.000, 0.000)

Figure S13 Total density of states and partial density of states of $Ba_2B_{10}O_{17}$.