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Syntheses, Crystal Structures and Characterizations of Three Alkaline Metal Borates

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Table S1 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Cs_2B_7O_9(OH)_5$, $K_2B_4O_5(OH)_4 \bullet H_2O$ and $K_2B_4O_5(OH)_4 \bullet 3.6H_2O$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

$Cs_2B_7O_9(OH)_5$	x	y	z	U(eq)	BVS
Cs(1)	265(1)	6587(1)	5662(1)	35(1)	1.03
Cs(2)	2250(1)	9882(1)	4184(1)	33(1)	0.96
B(1)	-427(8)	3934(6)	7018(4)	25(2)	3.09
B(2)	-2638(7)	10843(5)	2845(4)	22(1)	3.10
B(3)	4623(8)	12430(6)	5191(4)	23(2)	3.10
B(4)	2652(7)	11954(6)	6224(4)	25(2)	3.15
B(5)	4691(8)	6190(6)	5934(4)	26(2)	3.18
B(6)	5539(7)	11841(6)	3686(4)	22(1)	3.11
B(7)	-456(7)	7203(6)	8001(4)	25(2)	3.15
O(1)	5056(4)	11625(3)	4564(2)	22(1)	2.10
O(2)	4160(4)	7570(3)	3841(2)	23(1)	1.93
O(3)	2958(4)	12197(3)	5357(2)	23(1)	2.08
O(4)	1144(4)	4271(3)	7001(2)	27(1)	2.03
O(5)	-1081(5)	10521(4)	2830(3)	36(1)	1.19
O(6)	4210(4)	11445(3)	2835(2)	26(1)	1.86
O(7)	-1087(5)	8246(4)	3716(3)	41(1)	1.21
O(8)	4624(4)	13574(3)	4820(2)	23(1)	1.82
O(9)	1110(4)	6905(4)	7948(2)	34(1)	2.12
O(10)	4232(4)	6969(3)	6493(2)	28(1)	1.97
O(11)	2927(4)	8754(3)	6331(2)	28(1)	2.04
O(12)	-1583(5)	7247(5)	7136(3)	50(2)	1.26
O(13)	-1572(5)	4064(4)	6162(3)	42(1)	1.22
O(14)	4381(7)	5109(4)	6132(3)	44(1)	1.02

$K_2B_4O_5(OH)_4•H_2O$	x	y	z	U(eq)	BVS
K(1)	2068(1)	10902(1)	1999(1)	24(1)	1.10
K(2)	924(1)	6177(1)	1996(1)	26(1)	1.13
B(1)	5434(2)	2327(2)	3478(2)	15(1)	3.03
B(2)	2581(2)	6171(2)	-1492(2)	16(1)	3.00
B(3)	-2905(2)	10684(2)	1725(2)	16(1)	2.99
B(4)	-1482(2)	12625(2)	4323(2)	19(1)	3.04
O(1)	2517(1)	4484(1)	-137(1)	20(1)	1.19
O(2)	-2574(1)	9218(1)	1160(1)	23(1)	1.24
O(3)	3551(1)	2519(1)	4131(1)	20(1)	1.01
O(4)	183(1)	7657(2)	4441(1)	31(1)	1.17
O(5)	4571(1)	7332(1)	2495(1)	30(1)	0.25
O(6)	3063(1)	8033(2)	5241(1)	20(1)	1.87
O(7)	-1124(1)	13524(2)	2777(1)	20(1)	2.08
O(8)	5899(1)	10662(1)	2947(1)	18(1)	1.84
O(9)	5481(1)	4008(1)	2101(1)	15(1)	1.72
O(10)	2026(1)	7899(1)	-1038(1)	18(1)	2.03

$K_2B_4O_5(OH)_4•3.6H_2O$	x	y	z	U(eq)
K(1)	4450(1)	5252(1)	6306(1)	43(1)
K(2)	0	5848(1)	2500	62(1)
K(3)	5731(2)	2522(1)	7560(1)	48(1)
B(1)	2561(2)	7228(2)	5713(2)	21(1)
B(2)	1391(2)	5645(2)	5615(2)	22(1)
B(3)	6267(2)	3144(2)	5518(2)	21(1)
B(4)	1553(2)	6846(2)	4449(2)	20(1)
O(1)	1701(2)	7595(1)	5110(1)	20(1)
O(2)	711(2)	7174(1)	3835(1)	23(1)
O(4)	1121(2)	5859(1)	4819(1)	24(1)

O(5)	5211(2)	3182(2)	5942(1)	29(1)
O(6)	7284(2)	3329(1)	5949(1)	24(1)
O(7)	3726(2)	7059(1)	5301(1)	23(1)
O(8)	2711(2)	7923(2)	6392(1)	28(1)
O(9)	2132(2)	6238(1)	6066(1)	25(1)
O(10)	917(2)	5222(2)	974(1)	31(1)
O(11)	6487(2)	5407(2)	5325(2)	48(1)
O(12)	3539(4)	6592(2)	7641(2)	88(1)
O(13)	3714(4)	3900(4)	7508(3)	45(1)
O(14)	3124(8)	4551(5)	7693(3)	80(2)
O(15)	-1380(9)	4406(8)	1823(7)	69(3)
O(16)	6073(10)	1138(8)	7305(7)	70(3)

Table S2 Bond lengths [Å] and angles [deg] for $Cs_2B_7O_9(OH)_5$, $K_2B_4O_5(OH)_4•H_2O$ and $K_2B_4O_5(OH)_4•3.6H_2O$.

$Cs_2B_7O_9(OH)_5$			
B(1)-O(6)#1	1.337(7)	O(2)#1-B(7)-O(9)	122.3(5)
B(1)-O(13)	1.363(7)	O(12)-B(7)-O(9)	115.4(5)
B(1)-O(4)	1.379(7)	O(12)-Cs(1)-O(3)#3	70.29(12)
B(2)-O(11)#3	1.333(7)	O(12)-Cs(1)-O(13)#2	169.30(10)
B(2)-O(5)	1.362(7)	O(3)#3-Cs(1)-O(13)#2	99.68(11)
B(2)-O(4)#4	1.380(6)	O(12)-Cs(1)-O(9)	44.15(11)
B(3)-O(1)	1.411(7)	O(3)#3-Cs(1)-O(9)	112.28(9)
B(3)-O(8)	1.465(7)	O(13)#2-Cs(1)-O(9)	146.54(10)
B(3)-O(3)	1.490(7)	O(12)-Cs(1)-O(10)	111.11(12)
B(3)-O(2)#5	1.500(6)	O(3)#3-Cs(1)-O(10)	142.70(11)
B(4)-O(3)	1.339(7)	O(13)#2-Cs(1)-O(10)	79.06(11)
B(4)-O(7)#3	1.351(7)	O(9)-Cs(1)-O(10)	69.66(8)
B(4)-O(9)#6	1.369(6)	O(12)-Cs(1)-O(4)	84.64(13)
B(5)-O(10)	1.334(7)	O(3)#3-Cs(1)-O(4)	134.76(9)
B(5)-O(8)#5	1.350(7)	O(13)#2-Cs(1)-O(4)	100.72(12)
B(5)-O(14)	1.362(8)	O(9)-Cs(1)-O(4)	63.59(11)
B(6)-O(1)	1.414(6)	O(10)-Cs(1)-O(4)	80.98(9)
B(6)-O(10)#5	1.467(8)	O(12)-Cs(1)-O(7)	106.49(14)
B(6)-O(11)#5	1.471(7)	O(3)#3-Cs(1)-O(7)	41.85(9)
B(6)-O(6)	1.508(6)	O(13)#2-Cs(1)-O(7)	65.77(13)
B(7)-O(2)#1	1.327(6)	O(9)-Cs(1)-O(7)	135.62(13)
B(7)-O(12)	1.358(6)	O(10)-Cs(1)-O(7)	109.15(9)
B(7)-O(9)	1.375(7)	O(4)-Cs(1)-O(7)	160.03(10)
Cs(1)-O(12)	2.972(4)	O(12)-Cs(1)-O(11)	90.93(13)
Cs(1)-O(3)#3	3.104(4)	O(3)#3-Cs(1)-O(11)	102.19(12)

Cs(1)-O(13)#2	3.121(5)	O(13)#2-Cs(1)-O(11)	94.99(11)
Cs(1)-O(9)	3.158(5)	O(9)-Cs(1)-O(11)	69.49(9)
Cs(1)-O(10)	3.280(5)	O(10)-Cs(1)-O(11)	41.77(9)
Cs(1)-O(4)	3.338(5)	O(4)-Cs(1)-O(11)	115.65(10)
Cs(1)-O(7)	3.363(5)	O(7)-Cs(1)-O(11)	81.34(11)
Cs(1)-O(11)	3.404(5)	O(12)-Cs(1)-O(13)	76.51(14)
Cs(1)-O(13)	3.533(6)	O(3)#3-Cs(1)-O(13)	97.07(12)
Cs(2)-O(5)	3.081(5)	O(13)#2-Cs(1)-O(13)	101.72(10)
Cs(2)-O(1)	3.091(4)	O(9)-Cs(1)-O(13)	84.43(10)
Cs(2)-O(1)#5	3.096(4)	O(10)-Cs(1)-O(13)	119.86(9)
Cs(2)-O(3)	3.211(5)	O(4)-Cs(1)-O(13)	39.24(10)
Cs(2)-O(11)	3.244(5)	O(7)-Cs(1)-O(13)	126.10(10)
Cs(2)-O(2)	3.287(5)	O(11)-Cs(1)-O(13)	151.93(9)
Cs(2)-O(7)	3.345(5)	O(5)-Cs(2)-O(1)	118.63(13)
Cs(2)-O(6)	3.356(4)	O(5)-Cs(2)-O(1)#5	158.32(12)
O(6)#1-B(1)-O(13)	123.3(5)	O(1)-Cs(2)-O(1)#5	82.71(13)
O(6)#1-B(1)-O(4)	121.5(5)	O(5)-Cs(2)-O(3)	97.85(11)
O(13)-B(1)-O(4)	115.1(5)	O(1)-Cs(2)-O(3)	44.52(9)
O(11)#3-B(2)-O(5)	119.0(5)	O(1)#5-Cs(2)-O(3)	100.76(11)
O(11)#3-B(2)-O(4)#4	122.7(5)	O(5)-Cs(2)-O(11)	128.12(10)
O(5)-B(2)-O(4)#4	118.3(5)	O(1)-Cs(2)-O(11)	99.15(9)
O(1)-B(3)-O(8)	113.1(4)	O(1)#5-Cs(2)-O(11)	43.90(9)
O(1)-B(3)-O(3)	110.9(5)	O(3)-Cs(2)-O(11)	84.65(12)
O(8)-B(3)-O(3)	108.1(5)	O(5)-Cs(2)-O(2)	121.15(10)
O(1)-B(3)-O(2)#5	110.6(5)	O(1)-Cs(2)-O(2)	102.65(12)
O(8)-B(3)-O(2)#5	105.5(5)	O(1)#5-Cs(2)-O(2)	43.92(9)
O(3)-B(3)-O(2)#5	108.4(4)	O(3)-Cs(2)-O(2)	139.90(9)
O(3)-B(4)-O(7)#3	119.4(5)	O(11)-Cs(2)-O(2)	78.56(10)
O(3)-B(4)-O(9)#6	121.4(5)	O(5)-Cs(2)-O(7)	55.42(13)

O(7)#3-B(4)-O(9)#6	119.2(5)	O(1)-Cs(2)-O(7)	173.39(10)
O(10)-B(5)-O(8)#5	123.6(6)	O(1)#5-Cs(2)-O(7)	103.46(13)
O(10)-B(5)-O(14)	116.6(5)	O(3)-Cs(2)-O(7)	130.68(10)
O(8)#5-B(5)-O(14)	119.8(6)	O(11)-Cs(2)-O(7)	84.01(10)
O(1)-B(6)-O(10)#5	113.8(5)	O(2)-Cs(2)-O(7)	83.62(13)
O(1)-B(6)-O(11)#5	110.7(5)	O(5)-Cs(2)-O(6)	90.02(12)
O(10)#5-B(6)-O(11)#5	108.5(4)	O(1)-Cs(2)-O(6)	43.20(9)
O(1)-B(6)-O(6)	109.4(4)	O(1)#5-Cs(2)-O(6)	105.20(11)
O(10)#5-B(6)-O(6)	105.7(4)	O(3)-Cs(2)-O(6)	75.86(11)
O(11)#5-B(6)-O(6)	108.5(4)	O(11)-Cs(2)-O(6)	139.46(9)
O(2)#1-B(7)-O(12)	122.3(5)	O(2)-Cs(2)-O(6)	93.90(11)
O(7)-Cs(2)-O(6)	135.21(10)		

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,z+1/2 #2 -x,-y+1,-z+1 #3 -x,-y+2,-z+1 #4 x-1/2,-y+3/2,z-1/2

#5 -x+1,-y+2,-z+1 #6 -x+1/2,y+1/2,-z+3/2 #7 x+1/2,-y+3/2,z-1/2

#8 x+1/2,-y+3/2,z+1/2 #9 -x+1/2,y-1/2,-z+3/2

$K_2B_4O_5(OH)_4•H_2O$			
K(1)-O(5)	2.7898(6)	O(6)-K(1)-O(3)#1	70.12(3)
K(1)-O(8)	2.8391(11)	O(5)-K(1)-O(4)	71.34(2)
K(1)-O(1)#1	2.8590(9)	O(8)-K(1)-O(4)	115.14(2)
K(1)-O(2)#2	2.8795(11)	O(1)#1-K(1)-O(4)	161.78(2)
K(1)-O(10)#2	2.8918(10)	O(2)#2-K(1)-O(4)	114.98(3)
K(1)-O(7)	2.9093(11)	O(10)#2-K(1)-O(4)	73.30(2)
K(1)-O(6)	2.9200(10)	O(7)-K(1)-O(4)	83.91(3)
K(1)-O(3)#1	2.9993(10)	O(6)-K(1)-O(4)	43.83(2)
K(1)-O(4)	3.2651(12)	O(3)#1-K(1)-O(4)	104.24(3)
K(2)-O(7)#4	2.7308(10)	O(7)#4-K(2)-O(10)	124.64(3)

K(2)-O(10)	2.7573(10)	O(7)#4-K(2)-O(1)	83.50(3)
K(2)-O(1)	2.7707(10)	O(10)-K(2)-O(1)	52.13(3)
K(2)-O(4)	2.8126(12)	O(7)#4-K(2)-O(4)	103.02(3)
K(2)-O(2)	2.8686(7)	O(10)-K(2)-O(4)	127.76(3)
K(2)-O(3)	2.9702(7)	O(1)-K(2)-O(4)	167.021(19)
K(2)-O(5)	3.0761(8)	O(7)#4-K(2)-O(2)	91.41(3)
K(2)-O(9)	3.2543(10)	O(10)-K(2)-O(2)	87.67(3)
K(2)-O(1)#5	3.2680(8)	O(1)-K(2)-O(2)	122.02(3)
B(1)-O(9)	1.4481(17)	O(4)-K(2)-O(2)	69.55(3)
B(1)-O(3)	1.4503(17)	O(7)#4-K(2)-O(3)	72.87(3)
B(1)-O(6)#6	1.4959(17)	O(10)-K(2)-O(3)	117.88(3)
B(1)-O(8)#4	1.5045(18)	O(1)-K(2)-O(3)	77.14(2)
B(2)-O(1)	1.4435(17)	O(4)-K(2)-O(3)	93.89(3)
B(2)-O(9)#7	1.4701(18)	O(2)-K(2)-O(3)	154.37(3)
B(2)-O(7)#2	1.4881(18)	O(7)#4-K(2)-O(5)	149.81(3)
B(2)-O(10)	1.5091(18)	O(10)-K(2)-O(5)	74.19(2)
B(3)-O(10)#2	1.3623(18)	O(1)-K(2)-O(5)	94.63(2)
B(3)-O(8)#8	1.3709(19)	O(4)-K(2)-O(5)	74.042(18)
B(3)-O(2)	1.3829(18)	O(2)-K(2)-O(5)	114.43(2)
B(4)-O(6)#3	1.3564(19)	O(3)-K(2)-O(5)	77.33(2)
B(4)-O(7)	1.3586(19)	O(7)#4-K(2)-O(9)	108.12(3)
B(4)-O(4)#3	1.3856(18)	O(10)-K(2)-O(9)	75.03(3)
O(5)-K(1)-O(8)	68.35(3)	O(1)-K(2)-O(9)	55.20(2)
O(5)-K(1)-O(1)#1	126.47(2)	O(4)-K(2)-O(9)	111.85(2)
O(8)-K(1)-O(1)#1	78.71(2)	O(2)-K(2)-O(9)	159.00(3)
O(5)-K(1)-O(2)#2	74.88(2)	O(3)-K(2)-O(9)	45.00(2)
O(8)-K(1)-O(2)#2	100.76(2)	O(5)-K(2)-O(9)	49.78(2)
O(1)#1-K(1)-O(2)#2	71.24(3)	O(7)#4-K(2)-O(1)#5	45.65(3)
O(5)-K(1)-O(10)#2	126.07(3)	O(10)-K(2)-O(1)#5	85.19(3)

O(8)-K(1)-O(10)#2	165.58(3)	O(1)-K(2)-O(1)#5	70.540(17)
O(1)#1-K(1)-O(10)#2	90.82(2)	O(4)-K(2)-O(1)#5	122.02(2)
O(2)#2-K(1)-O(10)#2	84.95(2)	O(2)-K(2)-O(1)#5	65.62(3)
O(5)-K(1)-O(7)	154.13(3)	O(3)-K(2)-O(1)#5	111.76(3)
O(8)-K(1)-O(7)	118.26(3)	O(5)-K(2)-O(1)#5	159.297(19)
O(1)#1-K(1)-O(7)	78.85(3)	O(9)-K(2)-O(1)#5	123.25(2)
O(2)#2-K(1)-O(7)	124.26(3)	O(9)-B(1)-O(3)	111.55(11)
O(10)#2-K(1)-O(7)	49.09(3)	O(9)-B(1)-O(6)#6	110.02(11)
O(5)-K(1)-O(6)	59.61(2)	O(3)-B(1)-O(6)#6	109.02(11)
O(8)-K(1)-O(6)	72.04(3)	O(9)-B(1)-O(8)#4	107.98(11)
O(1)#1-K(1)-O(6)	144.33(3)	O(3)-B(1)-O(8)#4	109.71(10)
O(2)#2-K(1)-O(6)	133.56(3)	O(6)#6-B(1)-O(8)#4	108.51(11)
O(10)#2-K(1)-O(6)	113.55(3)	O(1)-B(2)-O(9)#7	111.28(11)
O(7)-K(1)-O(6)	97.26(3)	O(1)-B(2)-O(7)#2	108.47(11)
O(5)-K(1)-O(3)#1	108.24(2)	O(9)#7-B(2)-O(7)#2	110.04(11)
O(8)-K(1)-O(3)#1	48.80(3)	O(1)-B(2)-O(10)	110.69(11)
O(1)#1-K(1)-O(3)#1	75.36(2)	O(9)#7-B(2)-O(10)	109.21(11)
O(2)#2-K(1)-O(3)#1	138.88(2)	O(7)#2-B(2)-O(10)	107.05(11)
O(10)#2-K(1)-O(3)#1	119.13(3)	O(10)#2-B(3)-O(8)#8	122.51(13)
O(7)-K(1)-O(3)#1	70.03(3)	O(10)#2-B(3)-O(2)	118.44(13)
O(6)#3-B(4)-O(4)#3	116.41(13)	O(8)#8-B(3)-O(2)	119.05(12)
O(7)-B(4)-O(4)#3	119.57(13)	O(6)#3-B(4)-O(7)	124.02(13)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 -x,-y+2,-z #3 -x,-y+2,-z+1

#4 x,y-1,z #5 -x,-y+1,-z #6 -x+1,-y+1,-z+1

#7 -x+1,-y+1,-z #8 x-1,y,z #9 x+1,y,z

$K_2B_4O_5(OH)_4•3.6H_2O$			
K(1)-O(13)	2.772(5)	O(10)#3-K(2)-O(16)#4	71.8(2)

K(1)-O(11)	2.791(3)	O(15)-K(2)-O(16)#5	69.5(3)
K(1)-O(14)	2.866(6)	O(15)#3-K(2)-O(16)#5	22.8(3)
K(1)-O(5)	2.897(2)	O(10)-K(2)-O(16)#5	71.8(2)
K(1)-O(9)	2.914(2)	O(10)#3-K(2)-O(16)#5	77.9(2)
K(1)-O(12)	2.982(4)	O(16)#4-K(2)-O(16)#5	51.0(4)
K(1)-O(7)	2.990(2)	O(15)-K(2)-O(2)	153.0(2)
K(1)-O(11)#1	2.998(3)	O(15)#3-K(2)-O(2)	87.1(2)
K(1)-O(14)#2	3.295(9)	O(10)-K(2)-O(2)	137.97(6)
K(1)-O(12)#2	3.329(4)	O(10)#3-K(2)-O(2)	66.58(5)
K(1)-O(13)#2	3.332(5)	O(16)#4-K(2)-O(2)	137.4(2)
K(2)-O(15)	2.674(11)	O(16)#5-K(2)-O(2)	109.9(2)
K(2)-O(15)#3	2.674(11)	O(15)-K(2)-O(2)#3	87.1(2)
K(2)-O(10)	2.826(2)	O(15)#3-K(2)-O(2)#3	153.0(2)
K(2)-O(10)#3	2.826(2)	O(10)-K(2)-O(2)#3	66.58(5)
K(2)-O(16)#4	2.875(11)	O(10)#3-K(2)-O(2)#3	137.97(6)
K(2)-O(16)#5	2.875(11)	O(16)#4-K(2)-O(2)#3	109.9(2)
K(2)-O(2)	2.904(2)	O(16)#5-K(2)-O(2)#3	137.4(2)
K(2)-O(2)#3	2.904(2)	O(2)-K(2)-O(2)#3	106.74(8)
K(3)-O(16)	1.893(11)	K(3)#2-K(3)-O(16)	100.0(3)
K(3)-O(13)#2	1.908(6)	K(3)#2-K(3)-O(13)#2	108.37(15)
K(3)-O(16)#2	2.713(11)	O(16)-K(3)-O(13)#2	145.4(4)
K(3)-O(5)#2	2.810(3)	K(3)#2-K(3)-O(16)#2	43.4(2)
K(3)-O(8)#6	2.847(3)	O(16)-K(3)-O(16)#2	62.1(5)
K(3)-O(5)	2.851(3)	O(13)#2-K(3)-O(16)#2	150.9(3)
K(3)-O(13)	2.883(6)	K(3)#2-K(3)-O(5)#2	74.52(11)
K(3)-O(15)#7	2.885(11)	O(16)-K(3)-O(5)#2	124.2(3)
K(3)-O(14)#2	2.971(7)	O(13)#2-K(3)-O(5)#2	83.23(16)
K(3)-O(9)#6	3.215(2)	O(16)#2-K(3)-O(5)#2	81.7(2)
K(3)-O(6)	3.331(3)	K(3)#2-K(3)-O(8)#6	147.34(13)

B(1)-O(8)	1.447(3)	O(16)-K(3)-O(8)#6	98.8(3)
B(1)-O(1)	1.460(3)	O(13)#2-K(3)-O(8)#6	67.03(16)
B(1)-O(7)	1.482(3)	O(16)#2-K(3)-O(8)#6	130.4(2)
B(1)-O(9)	1.495(3)	O(5)#2-K(3)-O(8)#6	72.83(7)
B(2)-O(9)	1.354(3)	K(3)#2-K(3)-O(5)	71.76(10)
B(2)-O(4)	1.369(4)	O(16)-K(3)-O(5)	97.1(3)
B(2)-O(10)#9	1.382(3)	O(13)#2-K(3)-O(5)	74.11(16)
B(3)-O(6)	1.359(3)	O(16)#2-K(3)-O(5)	97.3(2)
B(3)-O(5)	1.368(3)	O(5)#2-K(3)-O(5)	130.23(9)
B(3)-O(7)#1	1.369(3)	O(8)#6-K(3)-O(5)	131.64(8)
B(4)-O(2)	1.442(3)	K(3)#2-K(3)-O(13)	38.90(10)
B(4)-O(1)	1.469(3)	O(16)-K(3)-O(13)	138.3(3)
B(4)-O(6)#1	1.470(3)	O(13)#2-K(3)-O(13)	70.2(2)
B(4)-O(4)	1.504(3)	O(16)#2-K(3)-O(13)	80.8(3)
O(13)-K(1)-O(11)	134.21(12)	O(5)#2-K(3)-O(13)	62.76(11)
O(13)-K(1)-O(14)	22.77(15)	O(8)#6-K(3)-O(13)	120.52(12)
O(11)-K(1)-O(14)	154.31(18)	O(5)-K(3)-O(13)	67.96(11)
O(13)-K(1)-O(5)	68.81(12)	K(3)#2-K(3)-O(15)#7	101.5(2)
O(11)-K(1)-O(5)	73.15(6)	O(16)-K(3)-O(15)#7	12.6(4)
O(14)-K(1)-O(5)	90.94(13)	O(13)#2-K(3)-O(15)#7	135.9(3)
O(13)-K(1)-O(9)	96.62(12)	O(16)#2-K(3)-O(15)#7	68.8(3)
O(11)-K(1)-O(9)	127.72(7)	O(5)#2-K(3)-O(15)#7	136.8(2)
O(14)-K(1)-O(9)	77.96(17)	O(8)#6-K(3)-O(15)#7	102.7(2)
O(5)-K(1)-O(9)	130.16(6)	O(5)-K(3)-O(15)#7	85.7(2)
O(13)-K(1)-O(12)	75.54(13)	O(13)-K(3)-O(15)#7	136.8(2)
O(11)-K(1)-O(12)	131.16(10)	K(3)#2-K(3)-O(14)#2	114.19(18)
O(14)-K(1)-O(12)	55.13(14)	O(16)-K(3)-O(14)#2	137.2(4)
O(5)-K(1)-O(12)	143.04(8)	O(13)#2-K(3)-O(14)#2	8.2(2)
O(9)-K(1)-O(12)	62.47(8)	O(16)#2-K(3)-O(14)#2	157.5(3)

O(13)-K(1)-O(7)	144.64(12)	O(5)#2-K(3)-O(14)#2	90.52(13)
O(11)-K(1)-O(7)	81.05(6)	O(8)#6-K(3)-O(14)#2	65.62(16)
O(14)-K(1)-O(7)	123.48(16)	O(5)-K(3)-O(14)#2	71.77(14)
O(5)-K(1)-O(7)	134.62(6)	O(13)-K(3)-O(14)#2	76.9(2)
O(9)-K(1)-O(7)	48.50(5)	O(15)#7-K(3)-O(14)#2	127.8(3)
O(12)-K(1)-O(7)	81.37(7)	K(3)#2-K(3)-O(9)#6	124.48(11)
O(13)-K(1)-O(11)#1	110.44(11)	O(16)-K(3)-O(9)#6	63.9(3)
O(11)-K(1)-O(11)#1	77.85(8)	O(13)#2-K(3)-O(9)#6	112.05(16)
O(14)-K(1)-O(11)#1	115.97(17)	O(16)#2-K(3)-O(9)#6	87.4(2)
O(5)-K(1)-O(11)#1	69.53(6)	O(5)#2-K(3)-O(9)#6	74.21(6)
O(9)-K(1)-O(11)#1	72.40(6)	O(8)#6-K(3)-O(9)#6	45.21(6)
O(12)-K(1)-O(11)#1	134.87(9)	O(5)-K(3)-O(9)#6	155.48(8)
O(7)-K(1)-O(11)#1	68.93(6)	O(13)-K(3)-O(9)#6	136.52(11)
O(13)-K(1)-O(14)#2	73.20(17)	O(15)#7-K(3)-O(9)#6	73.6(2)
O(11)-K(1)-O(14)#2	68.87(13)	O(14)#2-K(3)-O(9)#6	110.76(17)
O(14)-K(1)-O(14)#2	86.5(3)	K(3)#2-K(3)-O(6)	114.92(11)
O(5)-K(1)-O(14)#2	66.57(11)	O(16)-K(3)-O(6)	91.3(3)
O(9)-K(1)-O(14)#2	156.68(11)	O(13)#2-K(3)-O(6)	59.09(15)
O(12)-K(1)-O(14)#2	94.39(12)	O(16)#2-K(3)-O(6)	131.4(2)
O(7)-K(1)-O(14)#2	135.73(13)	O(5)#2-K(3)-O(6)	142.32(8)
O(11)#1-K(1)-O(14)#2	130.61(11)	O(8)#6-K(3)-O(6)	91.03(7)
O(13)-K(1)-O(12)#2	99.47(12)	O(5)-K(3)-O(6)	43.20(5)
O(11)-K(1)-O(12)#2	73.34(9)	O(13)-K(3)-O(6)	100.61(11)
O(14)-K(1)-O(12)#2	95.89(17)	O(15)#7-K(3)-O(6)	79.3(2)
O(5)-K(1)-O(12)#2	113.60(7)	O(14)#2-K(3)-O(6)	51.92(12)
O(9)-K(1)-O(12)#2	115.78(8)	O(9)#6-K(3)-O(6)	117.98(7)
O(12)-K(1)-O(12)#2	62.55(14)	O(8)-B(1)-O(1)	113.2(2)
O(7)-K(1)-O(12)#2	93.05(7)	O(8)-B(1)-O(7)	110.1(2)
O(11)#1-K(1)-O(12)#2	148.10(8)	O(1)-B(1)-O(7)	108.4(2)

O(14)#2-K(1)-O(12)#2	48.26(12)	O(8)-B(1)-O(9)	106.3(2)
O(13)-K(1)-O(13)#2	55.13(18)	O(1)-B(1)-O(9)	109.7(2)
O(11)-K(1)-O(13)#2	82.83(10)	O(7)-B(1)-O(9)	109.1(2)
O(14)-K(1)-O(13)#2	71.5(2)	O(8)-B(1)-K(1)	100.38(15)
O(5)-K(1)-O(13)#2	56.32(9)	O(1)-B(1)-K(1)	146.40(16)
O(9)-K(1)-O(13)#2	149.11(10)	O(7)-B(1)-K(1)	58.97(12)
O(12)-K(1)-O(13)#2	95.22(11)	O(9)-B(1)-K(1)	56.08(12)
O(7)-K(1)-O(13)#2	155.01(10)	O(9)-B(2)-O(4)	122.6(2)
O(11)#1-K(1)-O(13)#2	125.69(10)	O(9)-B(2)-O(10)#9	118.0(2)
O(14)#2-K(1)-O(13)#2	19.39(13)	O(4)-B(2)-O(10)#9	119.4(2)
O(12)#2-K(1)-O(13)#2	63.97(11)	O(6)-B(3)-O(5)	116.5(2)
O(15)-K(2)-O(15)#3	90.4(5)	O(6)-B(3)-O(7)#1	122.7(2)
O(15)-K(2)-O(10)	68.7(2)	O(5)-B(3)-O(7)#1	120.8(2)
O(15)#3-K(2)-O(10)	87.5(2)	O(2)-B(4)-O(1)	113.0(2)
O(15)-K(2)-O(10)#3	87.5(2)	O(2)-B(4)-O(6)#1	108.1(2)
O(15)#3-K(2)-O(10)#3	68.7(2)	O(1)-B(4)-O(6)#1	109.43(19)
O(10)-K(2)-O(10)#3	146.37(10)	O(2)-B(4)-O(4)	109.2(2)
O(15)-K(2)-O(16)#4	22.8(3)	O(1)-B(4)-O(4)	108.0(2)
O(15)#3-K(2)-O(16)#4	69.5(3)	O(6)#1-B(4)-O(4)	109.2(2)
O(10)-K(2)-O(16)#4	77.9(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,y,-z+3/2 #3 -x,y,-z+1/2 #4 -x+1/2,-y+1/2,z-1/2

#5 x-1/2,-y+1/2,-z+1 #6 x+1/2,y-1/2,-z+3/2 #7 -x+1/2,-y+1/2,z+1/2

#8 x-1/2,y+1/2,-z+3/2 #9 x,-y+1,z+1/2#10 x,-y+1,z-1/2

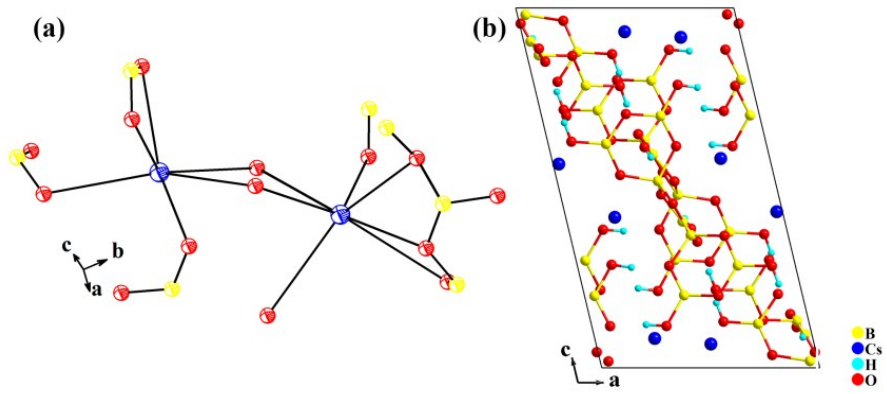

Figure S1 The asymmetric unit (a) and unit cell (b) of $Cs_2B_7O_9(OH)_5$.

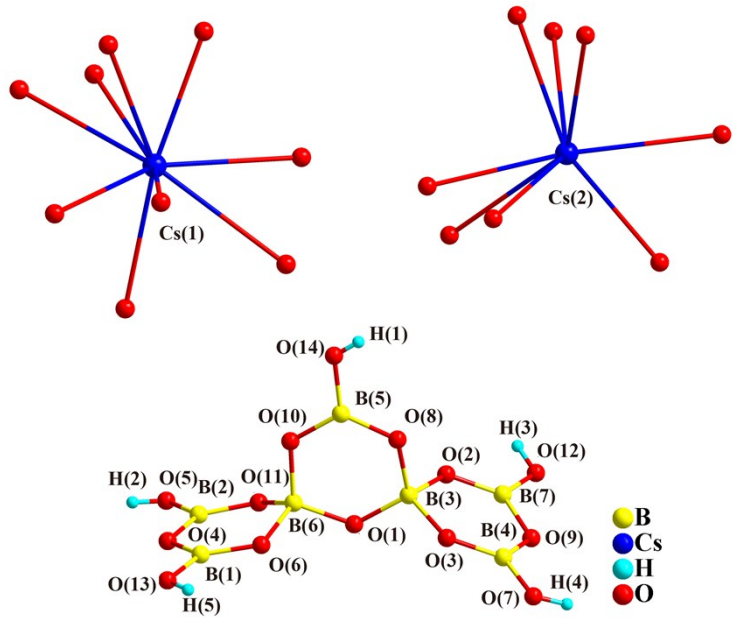

Figure S2 The coordination environments of cations in $Cs_2B_7O_9(OH)_5$.

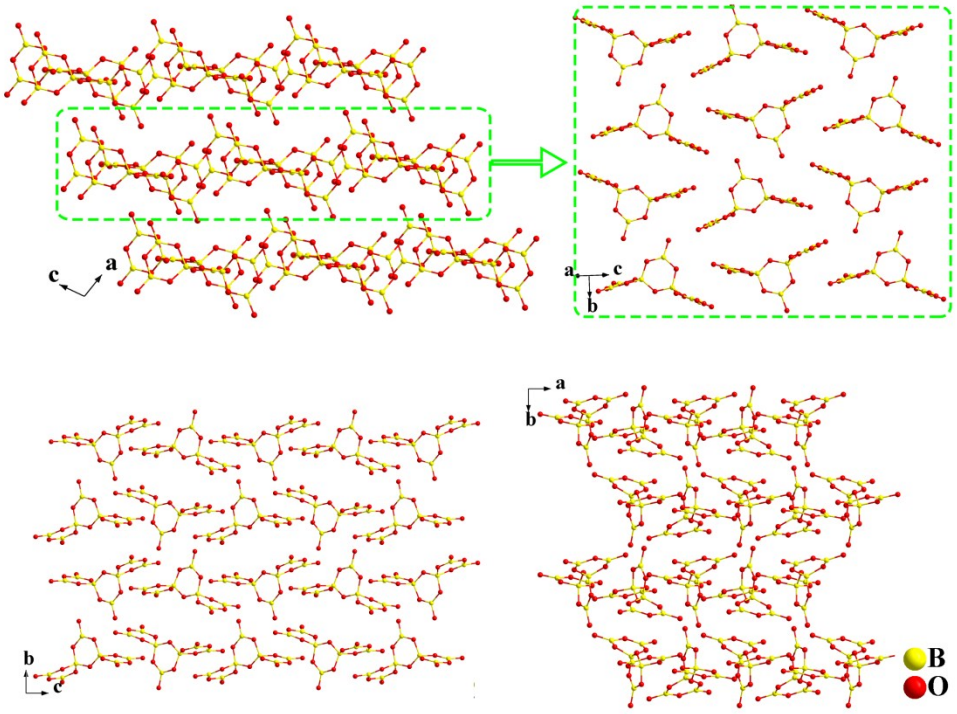

Figure S3 The arrangement of B_7O_{14} in $Cs_2B_7O_9(OH)_5$.

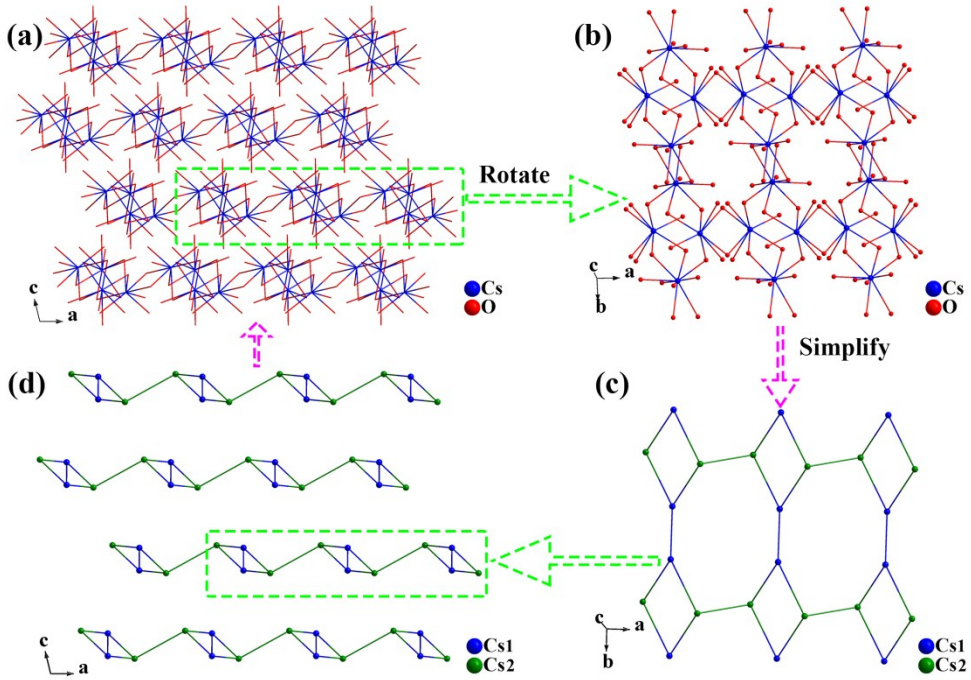

Figure S4 The arrangement of the Cs-O groups in $Cs_2B_7O_9(OH)_5$: (a) $[Cs_4O_{24}]_\infty$ layers; (b) a $[Cs_4O_{24}]_\infty$ layer; (c) simplified $[Cs_4O_{24}]_\infty$ layer regarding Cs-O groups as a node; (d) simplified $[Cs_4O_{24}]_\infty$ layers.

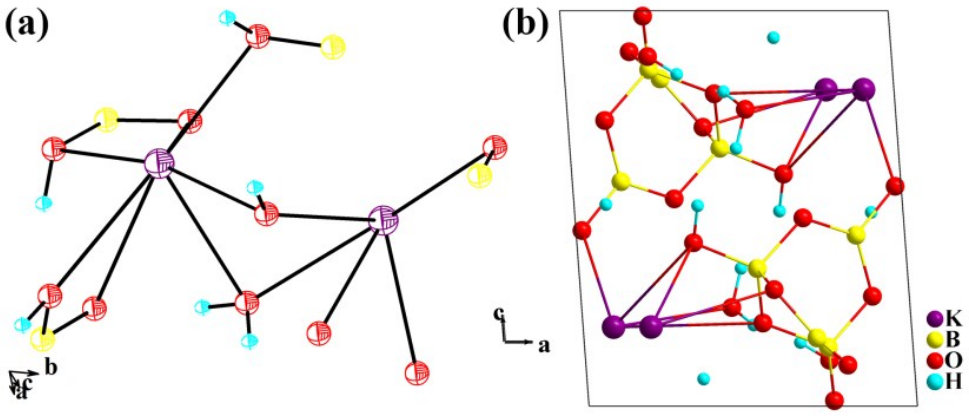

Figure S5 The asymmetric unit (a) and unit cell (b) of $K_2B_4O_5(OH)_4•H_2O$.

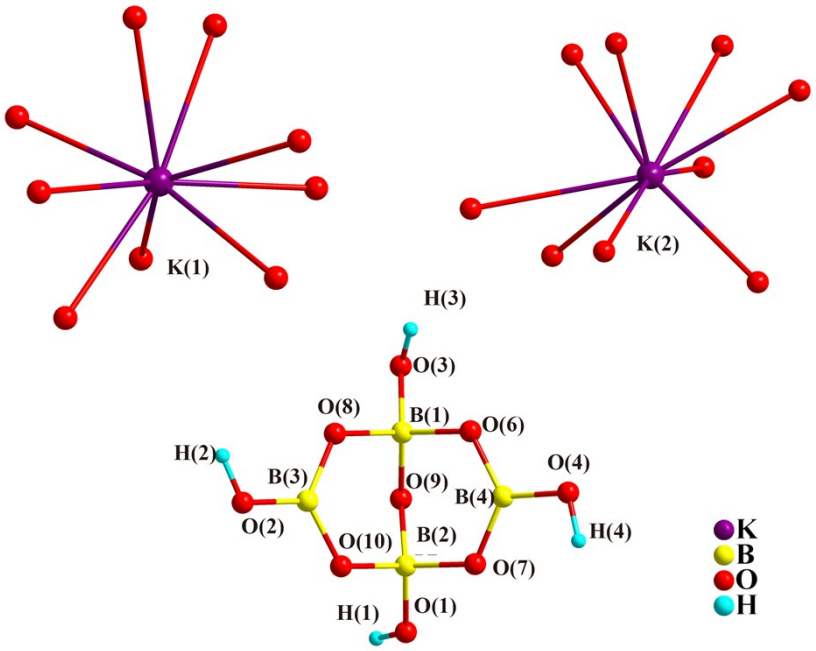

Figure S6 The coordination environments of cations in $K_2B_4O_5(OH)_4•H_2O$.

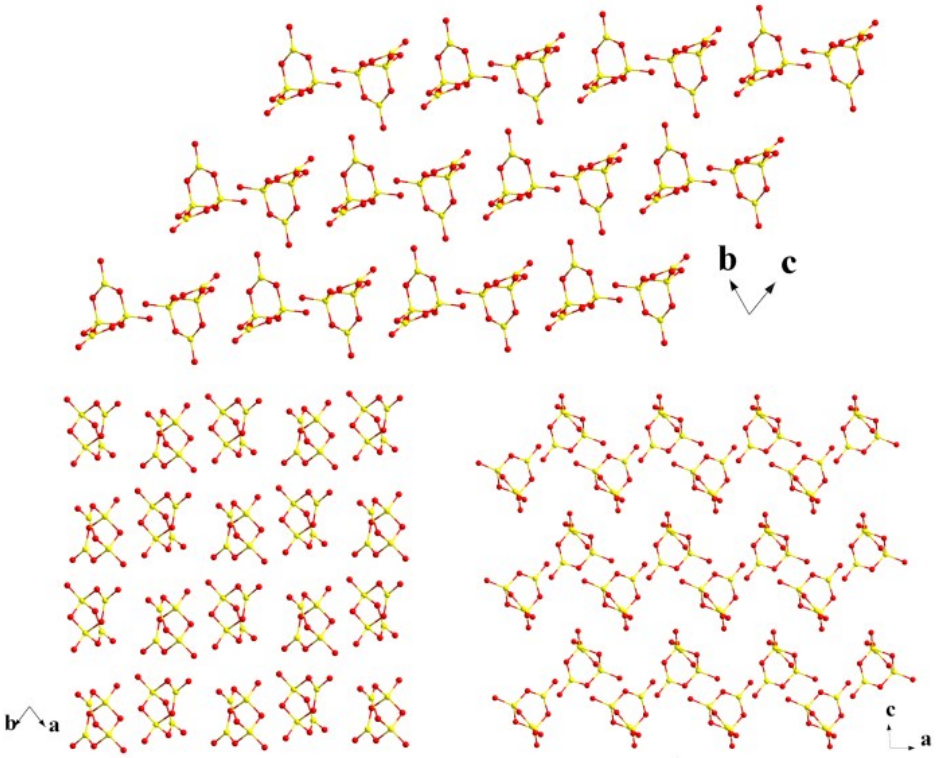

Figure S7 The arrangement of the B_4O_9 groups in $K_2B_4O_5(OH)_4 \cdot H_2O$.

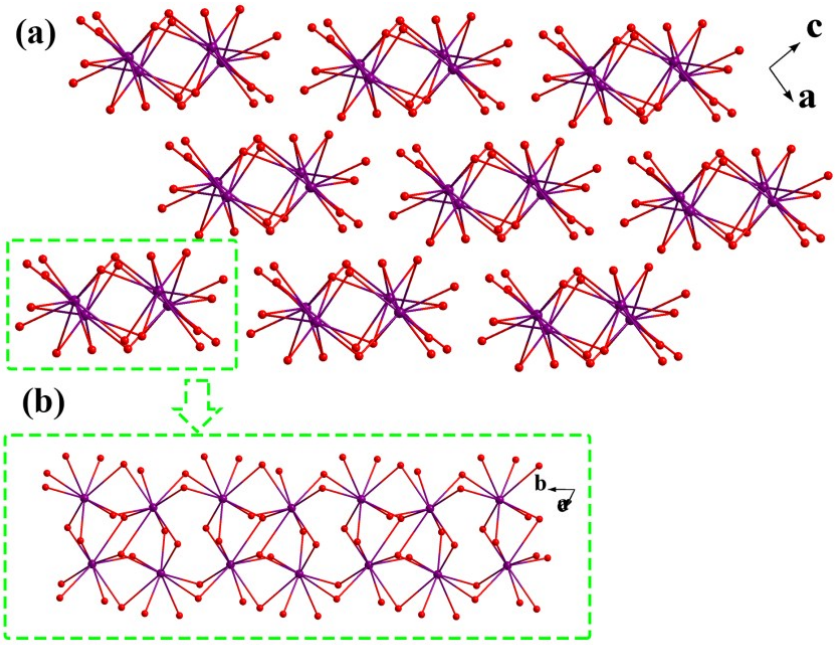

Figure S8 The $[K_4O_{20}]_\infty$ double chains in $K_2B_4O_5(OH)_4 \bullet H_2O$.

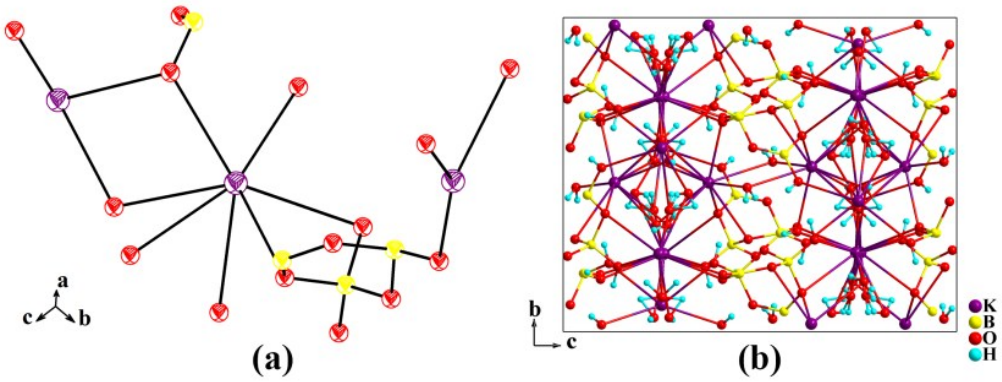

Figure S9 The asymmetric unit (a) and unit cell (b) of $K_2B_4O_5(OH)_4•3.6H_2O$.

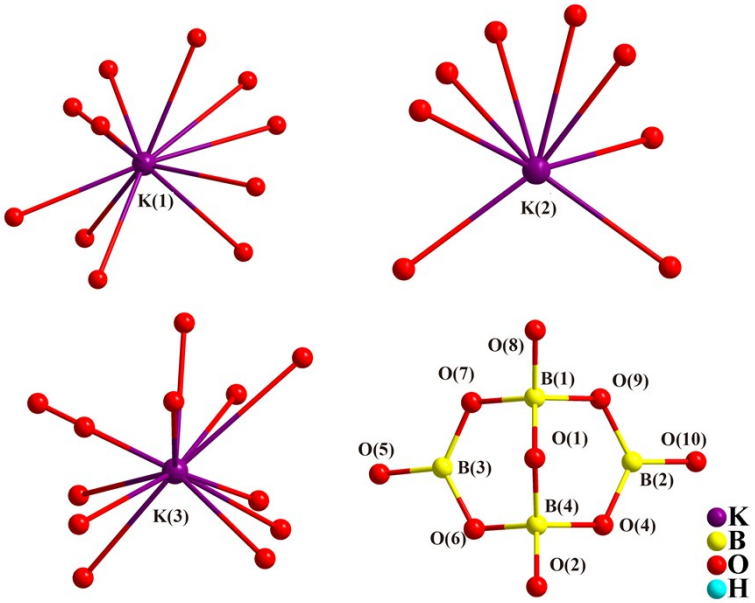

Figure S10 The coordination environments of cations in $K_2B_4O_5(OH)_4•3.6H_2O$.

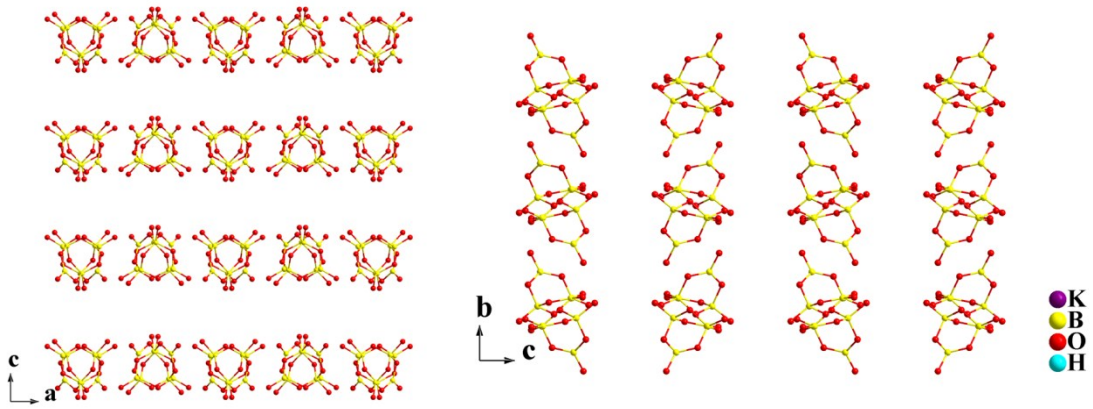

Figure S11 The arrangement of the B_4O_9 groups in $K_2B_4O_5(OH)_4•3.6H_2O$.

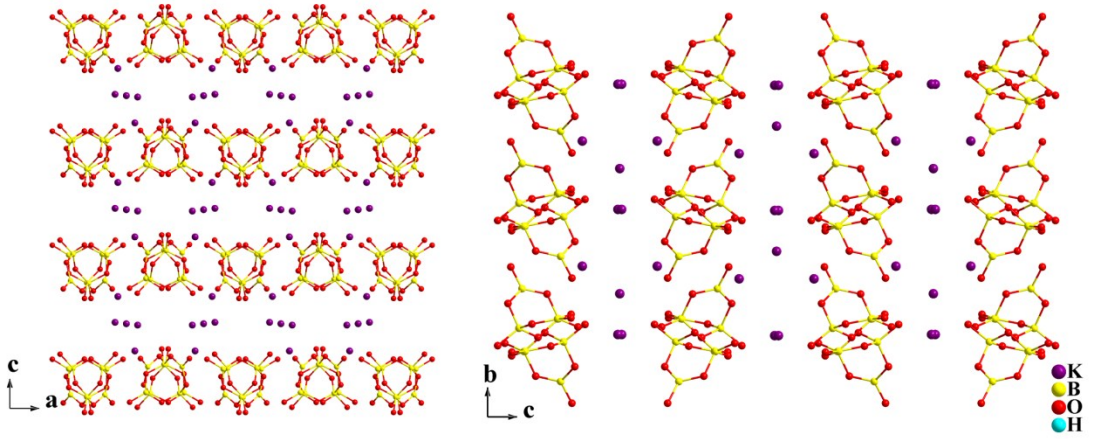

Figure S12 The K atoms located at the gaps of the B_4O_9 groups in $K_2B_4O_5(OH)_4•3.6H_2O$.

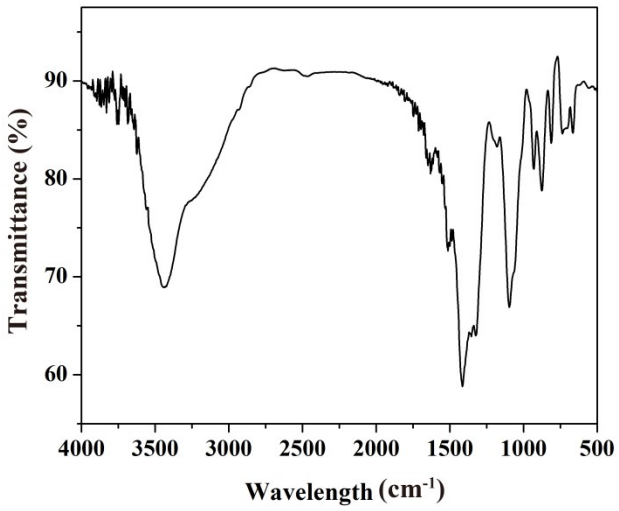

Figure S13 IR spectrum of $Cs_2B_7O_9(OH)_5$.

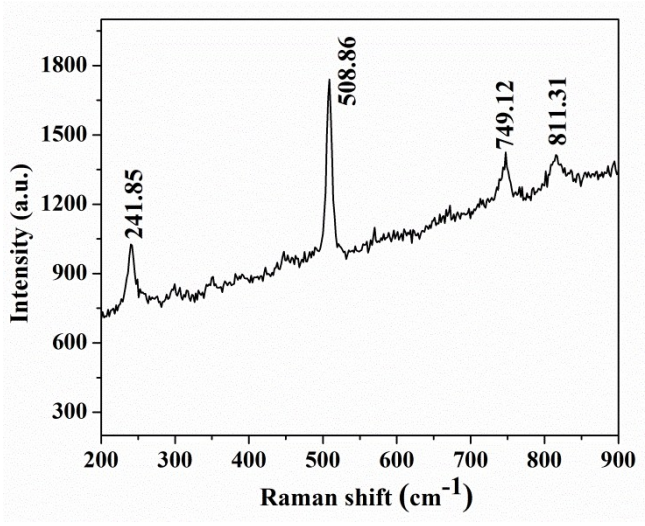

Figure S14 Raman spectrum of $Cs_2B_7O_9(OH)_5$.

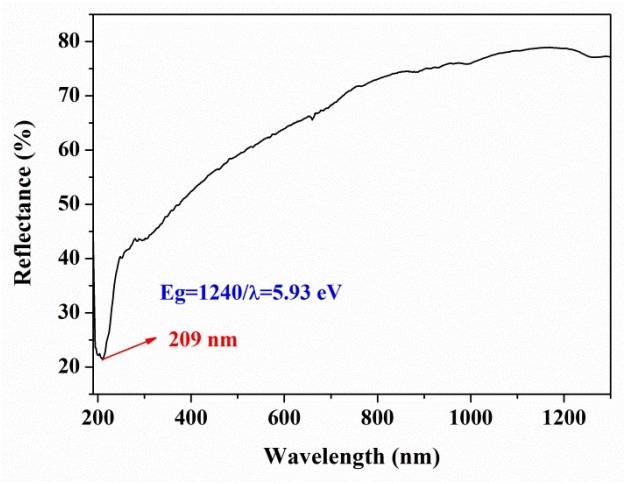

Figure S15 Diffuse reflectance spectrum of $Cs_2B_7O_9(OH)_5$.

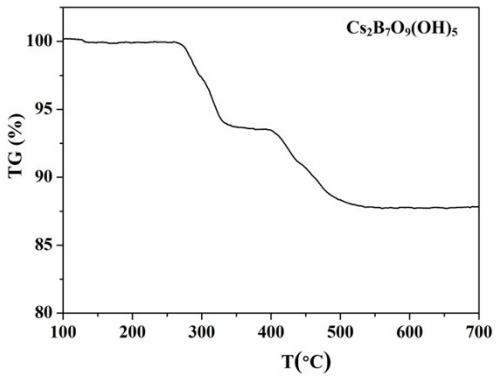

Figure S16 TG curve of the powder sample of $Cs_2B_7O_9(OH)_5$

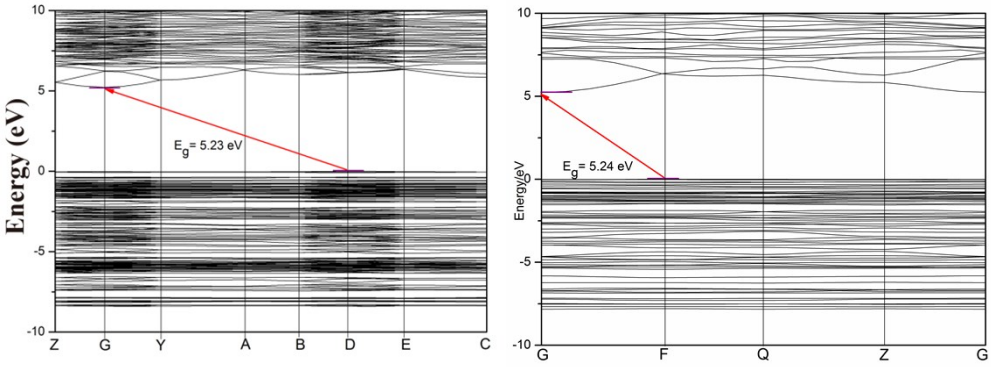

Figure S17 The band structures of $Cs_2B_7O_9(OH)_5$ (left) and $K_2B_4O_5(OH)_4 \cdot H_2O$(right).