Supporting Information

Hydroxyl-induced structural reconstruction: Two new potassium hepta-borates with deep-UV transparency and enhanced birefringence

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Table S1 Crystal data and structure refinement for $KB_7O_9(OH)_4$ and $KB_7O_{10}(OH)_2$.

Formula	$KB_7O_9(OH)_4$	$KB_7O_{10}(OH)_2$
Formula weight	326.80	308.79
Temperature	300(2) K	300(2) K
Wavelength	Mo Kα (λ = 0.71073 Å)	Mo Kα (λ = 0.71073 Å)
Crystal system	Monoclinic	Triclinic
Crystal description	block	
Crystal color	Colorless	
Space group	$P2_1/n$	$P\bar{1}$
a/Å	9.0346(6) Å	6.5675(17)
b/Å	4.2184(2)	6.5725(17)
c/Å	14.5266(9)	10.886(3)
α/°	90	101.240(9)
β/°	105.735(3)	94.162(9)
γ/°	90	91.591(9)
Volume	532.88(5) Å^3	459.2(2)
Z	2	2
ρ_{calc} g/cm^3	2.037	2.233
μ/mm^{-1}	0.571	0.648
F(000)	324	304
θ range/°	2.399 to 27.503	1.913 to 27.503
Index ranges	$-11 \le h \le 11$, $-5 \le k \le 5$, $-18 \le l \le 18$	$-8 \le h \le 8$, $-8 \le k \le 8$, $-12 \le l \le 14$
Reflns collected	8806	7842
Unique reflns (R_{int})	1228 (R_{int} = 0.0869)	2108(R_{int} = 0.0903)
Completeness	100%	99.9%
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/param	1228 / 0 / 106	2108 / 1 / 190
Goodness-of-fit on F^2	1.038	1.035
R_1[a)]/wR_2) [$I \ge 2\sigma(I)$]	0.0311/0.0657	0.0519/0.1082
R_1[a)]/wR_2) [all data]	0.0466/0.0700	0.0920/0.1357
Largest diff. peak/hole	0.218/0.257 e/Å^{-3}	0.51/-0.48 e/Å^{-3}

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w F_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$

Table S2 Atomic coordinates (× 10^4), equivalent isotropic displacement parameters (Å^2 × 10^3) and bond valence sum (BVS) calculation for $KB_7O_9(OH)_4$ and $KB_7O_{10}(OH)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)	BVS
			$KB_7O_9(OH)_4$		
K(1)	-2500	1933(1)	2500	32(1)	1.07
B(1)	238(2)	-1932(4)	3959(1)	16(1)	3.06
B(2)	2031(2)	1143(4)	3341(1)	15(1)	3.06
B(3)	2835(2)	-1483(5)	4912(1)	19(1)	3.03
B(4)	2500	6009(6)	2500	16(1)	3.06
O(1)	503(1)	125(3)	3315(1)	17(1)	2.1
O(2)	1345(1)	-2584(3)	4806(1)	18(1)	1.91
O(3)	3173(1)	293(3)	4219(1)	18(1)	1.83
O(4)	-1197(1)	6799(3)	3790(1)	21(1)	1.30
O(5)	2055(2)	4483(3)	3186(1)	22(1)	1.96
O(6)	2500	-619(4)	2500	14(1)	1.99
O(7)	3863(2)	-2258(4)	5744(1)	33(1)	1.12
			$KB_7O_{10}(OH)_2$		
K(1)	-3352.1(15)	8242.3(15)	2408.2(9)	30.7(3)	1.18
B(1)	-960(7)	7315(6)	5636(4)	19.4(9)	3.08
B(2)	1897(7)	7809(7)	4290(5)	24.0(10)	3.05
B(3)	5483(7)	7697(7)	5239(4)	19.4(9)	3.06
B(4)	6757(7)	7372(7)	7360(4)	18.8(9)	3.06
B(5)	6955(6)	5586(6)	9108(4)	17.1(9)	3.06
B(6)	7843(7)	3067(7)	10506(4)	19.5(9)	3.08
B(7)	7516(6)	-732(6)	9528(4)	18.4(9)	3.02
O(1)	-2573(4)	7614(4)	4819(2)	22.7(6)	2.13
O(2)	-1254(4)	7019(4)	6796(3)	24.0(6)	1.81
O(3)	994(4)	7271(4)	5283(3)	25.6(7)	2.02
O(4)	798(4)	8322(5)	3308(3)	28.5(7)	1.22
O(5)	3997(4)	7912(4)	4337(2)	22.2(6)	2.15
O(6)	5137(4)	7635(4)	6431(2)	21.6(6)	1.97
O(7)	6273(4)	5623(4)	7934(2)	20.7(6)	2.01
O(8)	6926(4)	3708(4)	9487(2)	22.7(6)	2.07
O(9)	8636(4)	4437(4)	11519(3)	23.8(6)	1.21
O(10)	7873(4)	971(4)	10489(2)	21.6(6)	2.04
O(11)	7629(4)	-2603(4)	9942(2)	19.7(6)	2.08
O(12)	7006(4)	-662(4)	8323(2)	20.5(6)	1.89

Table S3 Bond lengths (Å) and angles (deg) for $KB_7O_9(OH)_4$.

Bonds	Bond distances/angels (Å/˚)	Bonds	Bond angels (˚)
K(1)-O(1)#1	2.7568(11)	O(4)#3-K(1)-O(7)#4	71.64(4)
K(1)-O(1)	2.7569(11)	O(1)#1-K(1)-O(7)#5	102.80(3)
K(1)-O(4)	2.8136(13)	O(1)-K(1)-O(7)#5	78.63(3)
K(1)-O(4)#1	2.8136(13)	O(4)-K(1)-O(7)#5	109.03(4)
K(1)-O(4)#2	2.8973(13)	O(4)#2-K(1)-O(4)#3	83.24(5)
K(1)-O(4)#3	2.8973(13)	O(1)#1-K(1)-O(7)#4	78.63(3)
K(1)-O(7)#4	3.1224(15)	O(1)-K(1)-O(7)#4	102.80(3)
K(1)-O(7)#5	3.1224(15)	O(4)-K(1)-O(7)#4	67.04(4)
B(1)-O(1)	1.345(2)	O(4)#1-K(1)-O(7)#4	109.03(4)
B(1)-O(4)#3	1.362(2)	O(4)#2-K(1)-O(7)#4	112.37(4)
B(1)-O(2)	1.386(2)	O(4)#1-K(1)-O(7)#5	67.04(4)
B(2)-O(5)	1.428(2)	O(4)#2-K(1)-O(7)#5	71.64(4)
B(2)-O(6)	1.5824(19)	O(4)#3-K(1)-O(7)#5	112.37(4)
B(3)-O(7)	1.349(2)	O(7)#4-K(1)-O(7)#5	174.96(6)
O(1)#1-K(1)-O(1)	147.88(5)	O(1)-B(1)-O(4)#3	117.95(15)
O(1)#1-K(1)-O(4)	132.30(4)	O(1)-B(1)-O(2)	121.59(16)
O(1)-K(1)-O(4)	74.37(4)	O(4)#3-B(1)-O(2)	120.30(15)
O(1)#1-K(1)-O(4)#1	74.37(3)	O(5)-B(2)-O(1)	110.26(14)
O(1)-K(1)-O(4)#1	132.30(4)	O(5)-B(2)-O(3)	110.17(14)
O(4)-K(1)-O(4)#1	86.31(5)	O(1)-B(2)-O(3)	113.45(13)
O(1)#1-K(1)-O(4)#2	48.36(3)	O(5)-B(2)-O(6)	108.86(13)
O(1)-K(1)-O(4)#2	104.52(4)	O(1)-B(2)-O(6)	107.20(12)
O(4)-K(1)-O(4)#2	178.47(4)	O(3)-B(2)-O(6)	106.70(13)
O(4)#1-K(1)-O(4)#2	95.22(4)	O(7)-B(3)-O(3)	124.08(17)
O(1)#1-K(1)-O(4)#3	104.52(4)	O(7)-B(3)-O(2)	115.37(16)
O(1)-K(1)-O(4)#3	48.37(3)	O(3)-B(3)-O(2)	120.53(15)
O(4)-K(1)-O(4)#3	95.22(3)	O(5)-B(4)-O(5)#7	122.4(2)
O(4)#1-K(1)-O(4)#3	178.47(4)	O(5)-B(4)-O(6)#6	118.80(11)
		O(5)#7-B(4)-O(6)#6	118.80(11)
		$KB_7O_{10}(OH)_2$	
K(1)-O(1)	2.749(3)	O(5)#1-K(1)-O(8)#4	86.82(8)
K(1)-O(4)	2.824(3)	O(5)#1-K(1)-O(9)#5	112.93(9)
K(1)-O(5)#1	2.859(3)	O(5)#1-K(1)-O(10) #2	144.36(8)
K(1)-O(6)#3	3.061(3)	O(5)#1-K(1)-O(1)2#4	78.09(8)
K(1)-O(7)#4	3.087(3)	O(6)#3-K(1)-O(7)#4	115.57(8)
K(1)-O(8)#4	3.083(3)	O(6)#3-K(1)-O(8)#4	100.68(7)
K(1)-O(9)#5	2.884(3)	O(6)#3-K(1)-O(10) #2	79.89(7)

K(1)-O(10)#2	3.139(3)	O(7)#4-K(1)-O(1)0#2	130.90(8)
K(1)-O(11)#2	2.761(3)	O(8)#4-K(1)-O(7)#4	44.17(7)
K(1)-O(12)#4	3.058(3)	O(8)#4-K(1)-O(1)0#2	88.63(8)
B(1)-O(1)	1.377(5)	O(9)#5-K(1)-O(6)#3	174.34(8)
B(1)-O(2)	1.342(5)	O(9)#5-K(1)-O(7)#4	67.48(8)
B(1)-O(3)	1.365(5)	O(9)#5-K(1)-O(8)#4	84.80(8)
B(2)-O(3)	1.370(5)	O(9)#5-K(1)-O(10)#2	101.79(8)
B(2)-O(4)	1.349(6)	O(9)#5-K(1)-O(12)#4	139.90(8)
B(2)-O(5)	1.376(5)	O(11) #2-K(1)-O(4)	91.79(9)
B(3)-O(1)#6	1.386(5)	O(11)#2-K(1)-O(5)#1	152.25(8)
B(3)-O(5)	1.363(5)	O(11)#2-K(1)-O(6)#3	121.78(8)
B(3)-O(6)	1.342(5)	O(11)#2-K(1)-O(7)#4	93.61(8)
B(4)-O(2)#6	1.488(5)	O(11)#2-K(1)-O(8)#4	65.93(8)
B(4)-O(6)	1.451(5)	O(11)#2-K(1)-O(9)#5	61.67(8)
B(4)-O(7)	1.449(5)	O(11)#2-K(1)-O(10)#2	45.46(7)
B(4)-O(12)#7	1.494(5)	O(11)#2-K(1)-O(12)#4	90.28(8)
B(5)-O(7)	1.329(5)	O(12)#4-K(1)-O(6)#3	45.76(7)
B(5)-O(8)	1.375(5)	O(12)#4-K(1)-O(7)#4	88.05(8)
B(5)-O(11)#7	1.389(5)	O(12)#4-K(1)-O(8)#4	56.53(7)
B(6)-O(8)	1.368(5)	O(12)#4-K(1)-O(10)#2	70.04(7)
B(6)-O(9)	1.343(5)	O(2)-B(1)-O(1)	121.3(4)
B(6)-O(10)	1.375(5)	O(2)-B(1)-O(3)	117.7(4)
B(7)-O(10)	1.377(5)	O(3)-B(1)-O(1)	121.0(4)
B(7)-O(11)	1.391(5)	O(3)-B(2)-O(5)	118.1(4)
B(7)-O(12)	1.340(5)	O(4)-B(2)-O(3)	122.1(4)
O(1)-K(1)-O(4)	63.45(8)	O(4)-B(2)-O(5)	119.7(4)
O(1)-K(1)-O(5)#1	48.33(8)	O(5)-B(3)-O(1)#6	113.4(3)
O(1)-K(1)-O(6)#3	87.03(8)	O(6)-B(3)-O(1)#6	122.4(4)
O(1)-K(1)-O(7)#4	84.91(8)	O(6)-B(3)-O(5)	124.1(4)
O(1)-K(1)-O(8)#4	126.83(8)	O(2)#6-B(4)-O(12)#7	107.4(3)
O(1)-K(1)-O(9)#5	88.55(8)	O(6)-B(4)-O(2)#6	111.7(3)
O(1)-K(1)-O(1)0#2	144.08(8)	O(6)-B(4)-O(12)#7	107.8(3)
O(1)-K(1)-O(1)1#2	147.86(8)	O(7)-B(4)-O(2)#6	108.2(3)
O(1)-K(1)-O(1)2#4	121.68(8)	O(7)-B(4)-O(6)	110.8(3)
O(4)-K(1)-O(5)#1	111.45(9)	O(7)-B(4)-O(12)#7	110.9(3)
O(4)-K(1)-O(6)#3	108.31(8)	O(7)-B(5)-O(8)	118.2(3)
O(4)-K(1)-O(7)#4	123.66(9)	O(7)-B(5)-O(11)#7	121.0(3)
O(4)-K(1)-O(8)#4	150.03(8)	O(8)-B(5)-O(11)#7	120.8(4)
O(4)-K(1)-O(9)#5	66.46(9)	O(8)-B(6)-O(10)	118.3(4)
O(4)-K(1)-O(1)0#2	89.10(9)	O(9)-B(6)-O(8)	121.3(4)
O(4)-K(1)-O(1)2#4	147.98(9)	O(9)-B(6)-O(10)	120.3(4)
O(5)#1-K(1)-O(6)#3	66.34(8)	O(10)-B(7)-O(11)	112.8(3)

O(5)#1-K(1)-O(7)#4	61.26(7)	O(1)2-B(7)-O(10)	125.2(4)
		O(1)2-B(7)-O(11)	121.9(3)

Symmetry transformations used to generate equivalent atoms:

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

Table S4 Anisotropic Displacement Parameters ($Å^2×10^3$) for $KB_7O_9(OH)_4$ and $KB_7O_{10}(OH)_2$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
			$KB_7O_9(OH)_4$			
K(1)	27(1)	24(1)	36(1)	0	-7(1)	0
B(1)	19(1)	14(1)	17(1)	0(1)	7(1)	2(1)
B(2)	20(1)	12(1)	14(1)	0(1)	9(1)	-1(1)
B(3)	21(1)	19(1)	16(1)	0(1)	6(1)	-3(1)
B(4)	17(1)	12(1)	18(1)	0	4(1)	0
O(1)	16(1)	17(1)	19(1)	5(1)	6(1)	2(1)
O(2)	18(1)	21(1)	16(1)	3(1)	5(1)	-4(1)
O(3)	18(1)	20(1)	15(1)	0(1)	4(1)	-7(1)
O(4)	18(1)	25(1)	20(1)	4(1)	4(1)	-5(1)
O(5)	42(1)	9(1)	24(1)	1(1)	22(1)	1(1)
O(6)	19(1)	10(1)	15(1)	0	8(1)	0
O(7)	20(1)	52(1)	24(1)	15(1)	0(1)	-10(1)
			$KB_7O_{10}(OH)_2$			
K(1)	32.8(5)	39.7(6)	20.2(5)	5.8(4)	4.9(4)	7.2(4)
B(1)	22(2)	18(2)	18(2)	2.8(17)	2.7(17)	-0.4(16)
B(2)	25(2)	21(2)	25(2)	1.1(19)	1.2(19)	1.6(18)
B(3)	22(2)	20(2)	18(2)	8.5(17)	1.8(18)	0.6(17)
B(4)	21(2)	21(2)	15(2)	5.4(17)	3.6(17)	0.4(16)
B(5)	20(2)	13.8(19)	17(2)	0.4(17)	1.9(17)	-2.1(15)
B(6)	22(2)	17(2)	21(2)	6.0(17)	2.3(18)	0.0(16)
B(7)	18(2)	17(2)	20(2)	1.8(17)	3.8(17)	0.7(16)
O(1)	18.6(14)	30.5(15)	19.1(14)	6.3(12)	-0.8(11)	1.8(11)
O(2)	19.6(14)	30.4(15)	23.2(15)	7.6(12)	2.7(12)	2.3(11)
O(3)	18.2(14)	34.1(16)	27.2(16)	12.3(13)	2.5(12)	0.9(11)
O(4)	23.1(15)	38.2(17)	24.9(16)	8.5(14)	-1.0(13)	0.6(12)
O(5)	18.7(14)	29.0(15)	18.5(14)	3.6(12)	1.3(11)	1.4(11)
O(6)	18.2(13)	29.4(15)	17.9(13)	7.1(12)	-0.4(11)	-0.6(11)
O(7)	28.9(15)	15.5(13)	17.3(13)	3.0(11)	0.3(12)	-3.3(11)
O(8)	33.1(16)	11.6(12)	22.1(14)	3.1(11)	-4.6(12)	-1.7(11)
O(9)	32.7(16)	16.9(13)	19.5(14)	1.2(12)	-6.7(12)	-0.2(11)
O(10)	34.2(16)	10.9(12)	18.9(14)	1.8(11)	-1.6(12)	1.8(11)
O(11)	30.8(15)	11.8(12)	16.4(13)	3.7(10)	-0.7(11)	-1.6(10)
O(12)	30.5(15)	14.9(13)	16.3(13)	3.7(11)	1.5(12)	0.9(11)

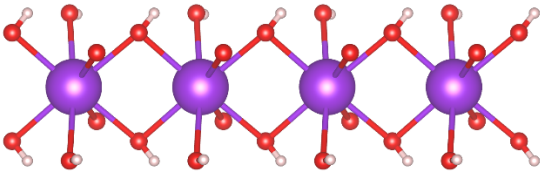

Figure S1 KO8 infinite chain of $KB_7O_9(OH)_4$.

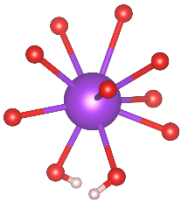

Figure S2 KO10 polyhedron of $KB_7O_{10}(OH)_2$.

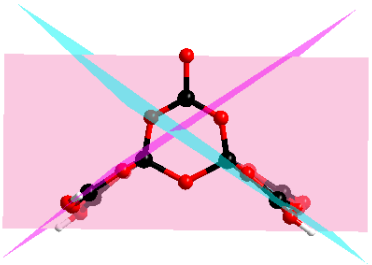

Figure S3 The planes of six-member rings of $[B_7O_{10}(OH)_4]$.

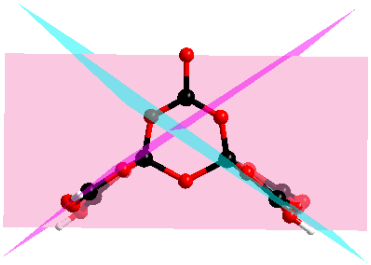

Figure S4 The planes of six-member rings of $[B_7O_{10}(OH)_2]$.