Supporting Information

Crystal Growth and Optical Properties of a Noncentrosymmetric Haloid Borate, $K_3B_6O_{10}Br$

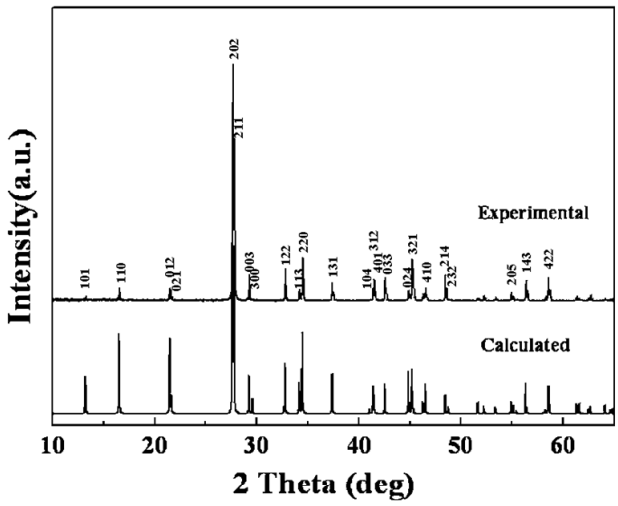

Figure S1. Experimental and calculated XRD patterns of the KBB.

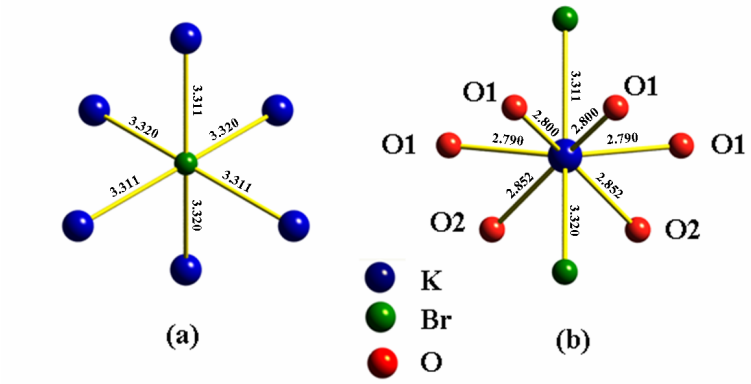

Figure S2. The coordinations and bond lengths (Å) of Br atoms (a), K atoms (b).

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for KBB. *Ueq* is defined as one third of the trace of the orthogonalized *Uij* tensor.

Atoms	Wyckoff positions	*x*	*y*	*z*	*Ueq*
K(1)	9*b*	0.84691(7)	0.15309(7)	0.20948(17)	0.0139(5)
B(1)	9*b*	0.7545(3)	0.2455(3)	-0.1300(7)	0.0049(12)
B(2)	9*b*	0.9656(7)	0.4828(3)	-0.0132(8)	0.0074(15)
O(1)	18*c*	0.8995(3)	0.3331(3)	-0.0483(3)	0.0082(7)
O(2)	9*b*	0.7782(2)	0.2218(2)	-0.2835(5)	0.0082(9)
O(3)	3*a*	0.6667	0.3333	-0.1232(8)	0.0017(14)
Br(1)	3*a*	0.6667	0.3333	0.32183(8)	0.0203(5)

Table S2. Selected bond lengths (Å) and angles (deg) for KBB.

K(1)-O(1)#1	2.793(3)	B(1)-O(2)	1.422(8)
K(1)-O(1)#2	2.793(3)	B(1)-O(1)	1.470(4)
K(1)-O(1)	2.801(3)	B(1)-O(1)#3	1.470(4)
K(1)-O(1)#3	2.801(3)	B(1)-O(3)	1.539(6)
K(1)-O(2)#4	2.853(3)		
K(1)-O(2) #5	2.853(3)	B(2)-O(1)	1.351(4)
K(1)-Br(1)	3.3111(14)	B(2)-O(1)#7	1.351(4)
K(1)-Br(1)#6	3.3207(15)	B(2)-O(2)#1	1.385(7)

Symmetry transformations used to generate equivalent atoms:

(#1) -*x*+*y*+5/3,-*x*+4/3,*z*+1/3; (#2) *x*-1/3,*x*-*y*-2/3,*z*+1/3; (#3) -y+1,-x+1,z; (#4) -y+4/3,x-y-1/3,z+2/3; (#5) -x+y+4/3,-x+2/3,z+2/3; (#6) x+1/3,y-1/3,z-1/3; (#7) x,x-y,z.

Table S3. Bond valence analysis of the KBB.[a,b]

Atom	O(1)	O(1)#1	O(2)	O(3)	Br(1)	Br(1)#1	$\sum_{cations}$
K(1)	$0.164^{[\times 2]}$	$0.169^{[\times 2]}$	$0.143^{[\times 2]}$		$^{[\times 3]}0.179$	$^{[\times 3]}0.175$	1.306
K(1)#1	$0.169^{[\times 2]}$	$0.164^{[\times 2]}$	$0.143^{[\times 2]}$		$^{[\times 3]}0.175$	$^{[\times 3]}0.179$	1.306
B(1)	0.766	0.766	0.848	$^{[\times 3]}0.636$			3.016
B(2)	1.063	1.063	0.951				3.077
$\sum_{anions}$	2.162	2.162	2.085	1.908	1.062	1.062	

[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: $S_i = \exp[(R_0-R_i)/B]$, where S_i = valence of bond "i", R_0 is a constant dependent upon the bonded elements, R_i is the bond length of bond i and B equals 0.37. Left and right superscripts indicate the number of equivalent bonds for anions and cations, respectively.