Supporting Information

$\text{K}_3\text{B}_6\text{O}_{10}\text{Cl}$: A New Structure Analogous to Perovskite with a Large SHG Response and Deep UV
Absorption Edge

Hongping Wu,^{†,‡} Shilie Pan,^{*,†} Kenneth R. Poeppelmeier,^{*,§} Hongyi Li,[†] Diansheng Jia,[‡]
Zhaohui Chen,[†] Xiaoyun Fan,[†] Yun Yang,[†] James M. Rondinelli,^δ Haosu Luo^ξ

[†]*Xinjiang Key Laboratory of Electronic Information Materials and Devices, Xinjiang
Technical Institute of Physics & Chemistry, Chinese Academy of Sciences, 40-1 South Beijing
Road, Urumqi 830011, China*

[‡]*College of Chemistry and Chemical Engineering, Xinjiang University, Urumqi 830046, China*

[§]*Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston IL
60208-3113, USA*

^δ*X-Ray Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne IL
60439, USA*

^ξ*State Key Laboratory of High Performance Ceramics and Superfine Microstructure,
Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 201800, China*

*To whom correspondence should be addressed. E-mail: slpan@ms.xjb.ac.cn (Shilie Pan);
krp@northwestern.edu (Kenneth R. Poeppelmeier).

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

Atom	x	y	z	U_{eq}
K(1)	-1795(1)	1795(1)	5627(1)	10(1)
Cl(1)	0	0	4405(1)	14(1)
B(1)	-874(1)	874(1)	8987(2)	4(1)
B(2)	1508(1)	3015(2)	7840(2)	5(1)
O(1)	-8(1)	2343(1)	8204(1)	6(1)
O(2)	2232(1)	4465(1)	7230(1)	6(1)
O(3)	0	0	8896(3)	3(1)

Table S2. Selected bond distances (Å) and angles (deg) for KBOC.

K(1)-O(1)#1	2.7621(9)	B(1)-O(2)#10	1.448(2)
K(1)-O(1)#2	2.7621(9)	B(1)-O(1)#3	1.4611(14)
K(1)-O(1)	2.7808(10)	B(1)-O(1)	1.4611(14)
K(1)-O(1)#3	2.7808(10)	B(1)-O(3)	1.5252(19)
K(1)-O(2)#4	2.8393(8)	B(2)-O(1)	1.3619(14)
K(1)-O(2)#2	2.8393(8)	B(2)-O(1)#11	1.3619(14)
K(1)-Cl(1)#5	3.2660(7)	B(2)-O(2)	1.373(2)
K(1)-Cl(1)	3.3101(6)	O(1)-K(1)-O(2)#2	115.43(3)
O(1)#1-K(1)-O(1)#2	150.33(4)	O(1)#3-K(1)-O(2)#2	157.49(3)
O(1)#1-K(1)-O(1)	125.02(4)	O(2)#4-K(1)-O(2)#2	71.65(5)
O(1)#2-K(1)-O(1)	75.952(15)	O(2)#10-B(1)-O(1)#3	110.94(10)
O(1)#1-K(1)-O(1)#3	75.952(15)	O(2)#10-B(1)-O(1)	110.94(10)
O(1)#2-K(1)-O(1)#3	125.02(4)	O(1)#3-B(1)-O(1)	107.02(15)
O(1)-K(1)-O(1)#3	49.97(4)	O(2)#10-B(1)-O(3)	108.90(16)
O(1)#1-K(1)-O(2)#4	49.81(3)	O(1)#3-B(1)-O(3)	109.51(10)
O(1)#2-K(1)-O(2)#4	119.09(3)	O(1)-B(1)-O(3)	109.51(10)
O(1)-K(1)-O(2)#4	157.49(3)	O(1)-B(2)-O(1)#11	121.21(17)
O(1)#3-K(1)-O(2)#4	115.43(3)	O(1)-B(2)-O(2)	119.24(8)
O(1)#1-K(1)-O(2)#2	119.09(3)	O(1)#11-B(2)-O(2)	119.24(8)
O(1)#2-K(1)-O(2)#2	49.81(3)	Cl(1)#5-K(1)-Cl(1)	164.19(3)
O(1)#1-K(1)-Cl(1)#5	101.95(2)	O(1)#1-K(1)-Cl(1)	80.91(2)

O(1)#2-K(1)-Cl(1)#5	101.95(2)	O(1)#2-K(1)-Cl(1)	80.91(2)
O(1)-K(1)-Cl(1)#5	81.44(2)	O(1)-K(1)-Cl(1)	84.24(2)
O(1)#3-K(1)-Cl(1)#5	81.44(2)	O(1)#3-K(1)-Cl(1)	84.24(2)
O(2)#4-K(1)-Cl(1)#5	79.06(3)	O(2)#4-K(1)-Cl(1)	113.41(3)
O(2)#2-K(1)-Cl(1)#5	79.06(3)	O(2)#2-K(1)-Cl(1)	113.41(3)

Note. Symmetry transformations used to generate equivalent atoms:

#1 $-x+y-2/3, y-1/3, z-1/3$ #2 $-y+1/3, x-y+2/3, z-1/3$
#3 $-y, -x, z$ #4 $x-2/3, y-1/3, z-1/3$ #5 $x-1/3, y+1/3, z+1/3$
#6 $-x+y-2/3, -x-1/3, z-1/3$ #7 $x+1/3, y-1/3, z-1/3$
#8 $-x+y, -x, z$ #9 $-y, x-y, z$ #10 $-x+y-1/3, -x+1/3, z+1/3$
#11 $-x+y, y, z$ #12 $x+2/3, y+1/3, z+1/3$

Captions for Figures:

Figure S1. Experimental and calculated XRD patterns of KBOC. The red curve is its experimental pattern, the black one is its calculated one.

Figure S2. The photograph of the KBOC (The minimum scale of the ruler is one millimeter.)

Figure S3. Potassium-coordinated environments in the crystal structure of compound.

Figure S4. The IR spectrum of KBOC.

Figure S5. TGA/DSC curve of KBOC.

Figure S6. (a) The point charge model of $[B_6O_{10}]$ group. The origin (0,0,0) for our dipole calculations is indicated. (Oxygen atoms (red) have $-2e$ charge and boron atoms (green) have $+3e$ charge.)

(b) The point charge model of $[ClK_6]$ group. The origin (0,0,0) for our dipole calculations is indicated. (Chlorine atoms (blue) have $-1e$ charge and potassium atoms (lavender) have $+1e$ charge)

Figure S7. The current vs temperature plot for KBOC.

Figure S1.

Figure S2.

Figure S3.

Figure S4.

Figure S5.

Figure S6.

Figure S7.

The measurements of pyroelectric and piezoelectric properties

Converse piezoelectric measurements were performed using a Radiant Technologies RT66A piezoelectric test system with a TREK (model 609C-6) high-voltage amplifier, Precision Materials Analyzer, Precision High Voltage Interface. The KBOC powder was pressed into 13-mm-diameter and 1.16-mm-thick pellet and sintered at 500 °C. Conducting silver paste was applied on both sides of the pellet surfaces for electrode. A maximum voltage of 2000 V was applied to the KBOC sample at room temperature. Although the crystallographic space group ($R3m$) permits a finite piezoelectric coefficient, we find d_{33} to be zero up to 10^{-12} C/N, suggesting that the KBOC sample has no piezoelectric response.

Pyroelectric measurements were performed using an Agilent 4294A precision impedance analyzer. In the measurement, the temperature of the sample was controlled by a Peltier heater and modulated sinusoidally with an amplitude of 1 °C at a frequency of 0.05 Hz. The pyroelectric current was amplified by an electrometer and the 90° out-of-phase component modulated with respect to the temperature was measured with a digital lock-in amplifier. The test curve is shown in Figure S7 in the Supporting Information. At room temperature (14°C), the measured pyroelectric coefficient (p) is 0.12 $\mu\text{C}/\text{m}^2\text{K}$. The coefficient (p) is so small, and we cannot prove that it is attributed to the pure pyroelectric coefficients. These may be the result of space charge.