Electronic Supplementary Material (ESI) for Dalton Transactions.

A new acentric borate-nitrate $Cs_3B_8O_{13}(NO_3)$ with interpenetrating porous 3D covalent and ionic lattices

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Experimental Section

Synthesis. Polycrystalline sample of $Cs_3B_8O_{13}(NO_3)$ (CBN) was synthesized by the conventional solid-state method. The starting material $CsNO_3$ was synthesized by the reaction of $CsCO_3$ (Tianjin Yaohua Chemical Reagent Co., Ltd., 99.0 %) and excess amount of HNO_3 (Aladdin AR, 40 wt %). Then, 5.847 g of as-synthesized $CsNO_3$ and 2.785 g of B_2O_3 (Aladdin Chemical Co., Ltd., 98 %) were thoroughly ground and placed into a silica tube which was sealed under 10^{-3} Pa. The silica tube was heated to 390 °C in 600 min in a muffle furnace, and held at this temperature for 5 days. Then turn off the muffle furnace and slowly bring it down to room temperature.

Single-Crystal Growth. Single crystal of CBN was grown by spontaneous crystallization in a sealed system. The mixture of $Mg(NO_3)_2·6H_2O$, CsF and B_2O_3 with molar ratio of 1:4:4 was evenly mixed into a silica tube and pumped to 10^{-3} Pa for sealing. The silica tube was slowly heated to 460 °C and held at this temperature for 2 days. Afterwards, it was cooled to 360 °C at a rate of 1 °C / h and then quickly drop to room temperature. The colorless crystals of CBN can be selected from the product.

Powder X-ray Diffraction. The powder XRD data were collected using the Bruker D2 PHASER X-ray diffractometer with Cu Kα radiation (λ = 1.5418 Å) in the range of 10-70 ° (2θ) with a fixed counting time and a scan step width of 1 s/step and 0.02 °.

Single Crystal X-ray Diffraction. A single crystal of CBN with good quality and appropriate size was chosen to obtain the diffraction data by Bruker SMART APEX II 4K CCD diffractometer using Mo Kα radiation (λ = 0.71073 Å) at 293 K. Then, the diffraction data were restored and corrected by SAINT and SCALE program, respectively.[1] The structure data is analyzed and refined by SHELXTL,[2] and the direct method is used for structure analysis. The correctness of the structure is determined by the PLATON program[3] and the international crystal society online testing website（http://checkcif.iucr.org/）.

Infrared Spectroscopy. The infrared (IR) spectrum was measured to specify the coordination of the B and N atoms. The IR spectrum was recorded on the ATR attachment of Thermo Scientific Nicolet iS50 FT-IR spectrometer in the range of 400-4000 cm^{-1}. The peak assignments are in agreements with the reported compounds.[4-6]

UV-vis-NIR Diffuse Reflectance Spectroscopy. To determine the cut-off edge of the title crystal, the UV-vis-NIR diffuse reflectance spectrum was recorded. The diffuse reflectance spectrum was measured at room temperature with a Shimadzu SolidSpec-3700DUV spectrophotometer.

TG-DSC Analyses. The thermal behavior of CBN was carried out on a NETZSCH STA 449C simultaneous analyzer instrument. The measurement was carried out from 160 to 800 °C with a heating rate of 10 °C·min^{-1} under flowing nitrogen gas.

SHG Measurement. Powder SHG measurement was carried out with the aid of Kurtz-Perry method[7] under the fundamental laser beam (λ = 1064 nm) emitted from a Q switched Nd:YAG laser. As the SHG efficiency strongly correlates with particle size, solidified polycrystalline sample of CBN was ground and standardized into below particle size ranges: 38-55, 55-88, 88-105, 105-155, and 155-200 μm. Polycrystalline KH_2PO_4 (KDP) samples of above sizes were employed as the standard materials.

Theoretical Calculations. The first principles calculation was carried out based on the density functional theory as implemented in the CASTEP package with the Generalized-Gradient-Approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional and the Norm

conservation pseudopotential.[8-12] The number of waves plane included in the basis was determined by cutoff energy of 830 eV. The interval of *k*-points is set to 0.04 $Å^{-1}$. And other calculation parameters and convergent criteria were the default values of the CASTEP code. When calculating the optical properties, we added 2.463 eV scissors operator to move the calculated bandgap to be equivalent to the experimental bandgap. The following orbital electrons were treated as valence electrons: B-2*s*2*p*, N-2*s*2*p*, O-2*s*2*p*, Cs-5*s*5*p*6*s*. Complex dielectric function $(\omega) = \varepsilon(\omega) + i\varepsilon(\omega)$ was used to calculate the linear optical properties.[13] The imaginary part of dielectric function ε can be calculated on the basis of the electronic structures and the real part was determined by the Kramers-Kronig transform. According to this result, the refractive index and thus the birefringence Δn can be obtained.

Table S1. Crystal data and structure refinement for CBN.

Empirical formula	$Cs_3B_8O_{13}(NO_3)$
Formula weight	755.22
Temperature / K	296(2)
Crystal system	Orthorhombic
Space group	$Pca2_1$
a / Å	8.785(6)
b / Å	13.001(9)
c / Å	14.593(10)
Volume / Å	1667(2)
Z, ρ_{calcd} / $g \cdot cm^{-3}$	4, 3.010
Theta range for data collection/°	2.792 to 27.446
Reflections collected / unique	9809 / 3553 [R(int) = 0.0807]
Completeness	99.9 %
Goodness-of-fit on F^2	0.944
Final R indices [$I > 2\sigma(I)$][a]	$R_1 = 0.0475$, $wR_2 = 0.0829$
R indices (all data)[a]	$R_1 = 0.0751$, $wR_2 = 0.0943$
Largest diff. peak and hole / $e \cdot Å^{-3}$	1.158 and – 1.021

[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 ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and bond valence sums (BVS)[14-15] for CBN. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	Wyck.	*x/a*	*y/b*	*z/c*	*U*(eq)	BVS
Cs(1)	4a	4862(1)	4768(1)	4726(1)	31(1)	1.10
Cs(2)	4a	6135(1)	7643(1)	2641(1)	32(1)	0.91
Cs(3)	4a	4347(1)	10152(1)	5001(1)	34(1)	1.10
B(1)	4a	-300(20)	4325(15)	7244(13)	19(4)	3.02
B(2)	4a	2180(20)	5075(15)	7278(16)	20(4)	3.05
B(3)	4a	2780(20)	6504(14)	6250(13)	20(4)	3.09
B(4)	4a	2110(20)	8357(15)	6146(13)	16(4)	3.11
B(5)	4a	2470(30)	7371(14)	4762(16)	20(4)	3.03
B(6)	4a	2020(20)	8175(14)	3331(13)	15(4)	3.00
B(7)	4a	20(20)	9250(13)	2680(13)	16(4)	3.04
B(8)	4a	2740(20)	9651(15)	2400(14)	22(5)	3.08
N(1)	4a	7310(20)	7450(13)	4996(12)	41(5)	5.00
O(1)	4a	-618(12)	3703(9)	6551(8)	26(3)	1.93
O(2)	4a	1164(12)	4360(8)	7618(9)	21(2)	2.08
O(3)	4a	3600(14)	5075(8)	7668(9)	23(3)	2.12
O(4)	4a	1773(13)	5716(8)	6600(8)	26(3)	2.01
O(5)	4a	2320(14)	7504(9)	6636(8)	26(3)	1.96
O(6)	4a	2748(13)	6509(7)	5256(7)	21(3)	2.24
O(7)	4a	6934(17)	6660(10)	4602(12)	51(4)	2.24
O(8)	4a	8450(20)	7460(12)	5504(13)	66(6)	2.02
O(9)	4a	6616(17)	8274(11)	4817(13)	66(5)	2.00
O(10)	4a	1803(12)	9294(8)	6474(7)	20(3)	2.11
O(11)	4a	2157(12)	8289(8)	5182(9)	23(3)	2.22
O(12)	4a	2397(13)	7310(8)	3822(8)	23(3)	1.98
O(13)	4a	3089(12)	8878(8)	3105(8)	19(3)	2.04
O(14)	4a	1123(13)	9900(8)	2350(9)	21(3)	1.98
O(15)	4a	-1460(12)	9396(8)	2615(10)	24(3)	2.17
O(16)	4a	491(11)	8350(8)	3144(7)	20(3)	1.91

Table S3. Bond lengths (Å) and angles (°) for CBN.

Cs(1)-O(6)	3.029(10)	O(14)#7-Cs(2)-O(9)	83.1(3)
Cs(1)-O(7)	3.066(14)	O(15)#5-Cs(2)-O(5)#3	130.1(3)
Cs(1)-O(6)#1	3.127(11)	O(8)#6-Cs(2)-O(5)#3	70.8(4)
Cs(1)-O(7)#2	3.177(14)	O(13)-Cs(2)-O(5)#3	50.6(3)
Cs(1)-O(2)#3	3.249(14)	O(7)-Cs(2)-O(5)#3	124.2(3)
Cs(1)-O(4)#1	3.270(12)	O(14)#7-Cs(2)-O(5)#3	89.6(3)
Cs(1)-O(3)#4	3.299(13)	O(9)-Cs(2)-O(5)#3	123.0(3)
Cs(1)-O(8)#2	3.350(17)	O(15)#5-Cs(2)-O(2)#4	94.8(3)
Cs(1)-O(1)#1	3.350(12)	O(8)#6-Cs(2)-O(2)#4	81.7(4)
Cs(2)-O(15)#5	3.108(11)	O(13)-Cs(2)-O(2)#4	159.7(3)
Cs(2)-O(8)#6	3.150(19)	O(7)-Cs(2)-O(2)#4	64.4(4)
Cs(2)-O(13)	3.194(11)	O(14)#7-Cs(2)-O(2)#4	137.2(3)
Cs(2)-O(7)	3.211(16)	O(9)-Cs(2)-O(2)#4	96.1(3)
Cs(2)-O(14)#7	3.223(11)	O(5)#3-Cs(2)-O(2)#4	124.2(3)
Cs(2)-O(9)	3.306(19)	O(15)#5-Cs(2)-O(3)#4	133.4(3)
Cs(2)-O(5)#3	3.376(12)	O(8)#6-Cs(2)-O(3)#4	85.9(3)
Cs(2)-O(2)#4	3.522(11)	O(13)-Cs(2)-O(3)#4	123.7(3)
Cs(2)-O(3)#4	3.541(10)	O(7)-Cs(2)-O(3)#4	65.1(3)
Cs(2)-O(12)	3.734(12)	O(14)#7-Cs(2)-O(3)#4	172.2(3)
Cs(3)-O(11)	3.104(11)	O(9)-Cs(2)-O(3)#4	103.2(3)
Cs(3)-O(10)#7	3.129(10)	O(5)#3-Cs(2)-O(3)#4	90.6(3)
Cs(3)-O(9)	3.163(14)	O(2)#4-Cs(2)-O(3)#4	38.6(3)
Cs(3)-O(9)#8	3.165(15)	O(15)#5-Cs(2)-O(12)	133.5(3)
Cs(3)-O(11)#7	3.204(10)	O(8)#6-Cs(2)-O(12)	123.4(4)
Cs(3)-O(8)#8	3.286(16)	O(13)-Cs(2)-O(12)	39.1(3)
Cs(3)-O(10)	3.296(11)	O(7)-Cs(2)-O(12)	74.6(3)
Cs(3)-O(13)	3.409(11)	O(14)#7-Cs(2)-O(12)	100.0(3)
Cs(3)-O(14)#9	3.469(13)	O(9)-Cs(2)-O(12)	72.4(3)
Cs(3)-O(16)#7	3.485(11)	O(5)#3-Cs(2)-O(12)	53.4(2)
B(1)-O(1)	1.32(2)	O(2)#4-Cs(2)-O(12)	120.7(2)
B(1)-O(3)#2	1.39(2)	O(3)#4-Cs(2)-O(12)	86.4(3)
B(1)-O(2)	1.40(2)	O(11)-Cs(3)-O(10)#7	123.3(3)
B(2)-O(4)	1.34(2)	O(11)-Cs(3)-O(9)	78.2(3)
B(2)-O(3)	1.38(2)	O(10)#7-Cs(3)-O(9)	78.6(4)
B(2)-O(2)	1.38(2)	O(11)-Cs(3)-O(9)#8	92.4(3)
B(3)-O(4)	1.45(2)	O(10)#7-Cs(3)-O(9)#8	115.6(4)
B(3)-O(6)	1.45(2)	O(9)-Cs(3)-O(9)#8	165.8(5)
B(3)-O(5)	1.48(2)	O(11)-Cs(3)-O(11)#7	164.5(4)
B(3)-O(1)#1	1.49(2)	O(10)#7-Cs(3)-O(11)#7	42.8(3)
B(4)-O(5)	1.33(2)	O(9)-Cs(3)-O(11)#7	90.6(4)
B(4)-O(10)	1.34(2)	O(9)#8-Cs(3)-O(11)#7	100.5(3)
B(4)-O(11)	1.41(2)	O(11)-Cs(3)-O(8)#8	124.7(4)
B(5)-O(6)	1.36(2)	O(10)#7-Cs(3)-O(8)#8	78.2(3)

B(5)-O(11)	1.37(2)	O(9)-Cs(3)-O(8)#8	154.1(4)
B(5)-O(12)	1.38(3)	O(9)#8-Cs(3)-O(8)#8	39.3(4)
B(6)-O(13)	1.35(2)	O(11)#7-Cs(3)-O(8)#8	64.5(4)
B(6)-O(12)	1.37(2)	O(11)-Cs(3)-O(10)	42.3(3)
B(6)-O(16)	1.39(2)	O(10)#7-Cs(3)-O(10)	95.6(3)
B(7)-O(15)	1.31(2)	O(9)-Cs(3)-O(10)	102.8(4)
B(7)-O(14)	1.38(2)	O(9)#8-Cs(3)-O(10)	76.1(4)
B(7)-O(16)	1.41(2)	O(11)#7-Cs(3)-O(10)	133.1(3)
B(8)-O(14)	1.46(2)	O(8)#8-Cs(3)-O(10)	90.6(4)
B(8)-O(15)#7	1.46(2)	O(11)-Cs(3)-O(13)	59.3(3)
B(8)-O(13)	1.47(2)	O(10)#7-Cs(3)-O(13)	153.2(3)
B(8)-O(10)#3	1.48(2)	O(9)-Cs(3)-O(13)	76.1(4)
N(1)-O(7)	1.223(19)	O(9)#8-Cs(3)-O(13)	90.0(4)
N(1)-O(8)	1.24(2)	O(11)#7-Cs(3)-O(13)	128.6(3)
N(1)-O(9)	1.26(2)	O(8)#8-Cs(3)-O(13)	124.2(3)
O(6)-Cs(1)-O(7)	77.3(4)	O(10)-Cs(3)-O(13)	98.3(3)
O(6)-Cs(1)-O(6)#1	146.2(4)	O(11)-Cs(3)-O(14)#9	76.6(3)
O(7)-Cs(1)-O(6)#	187.7(3)	O(10)#7-Cs(3)-O(14)#9	54.9(3)
O(6)-Cs(1)-O(7)#	287.4(3)	O(9)-Cs(3)-O(14)#9	94.9(4)
O(7)-Cs(1)-O(7)#2	161.1(4)	O(9)#8-Cs(3)-O(14)#9	93.1(4)
O(6)#1-Cs(1)-O(7)#2	111.1(3)	O(11)#7-Cs(3)-O(14)#9	94.0(3)
O(6)-Cs(1)-O(2)#3	101.2(3)	O(8)#8-Cs(3)-O(14)#9	80.8(4)
O(7)-Cs(1)-O(2)#3	103.9(4)	O(10)-Cs(3)-O(14)#9	40.8(3)
O(6)#1-Cs(1)-O(2)#3	111.9(3)	O(11)-Cs(3)-O(16)#7	132.9(3)
O(7)#2-Cs(1)-O(2)#3	68.0(4)	O(10)#7-Cs(3)-O(16)#7	101.9(3)
O(6)-Cs(1)-O(4)#1	104.2(3)	O(9)-Cs(3)-O(16)#7	100.6(4)
O(7)-Cs(1)-O(4)#1	84.2(4)	O(9)#8-Cs(3)-O(16)#7	78.0(4)
O(6)#1-Cs(1)-O(4)#1	43.5(3)	O(11)#7-Cs(3)-O(16)#7	59.2(3)
O(7)#2-Cs(1)-O(4)#1	110.5(3)	O(8)#8-Cs(3)-O(16)#7	73.5(4)
O(2)#3-Cs(1)-O(4)#1	154.5(3)	O(10)-Cs(3)-O(16)#7	153.1(2)
O(6)-Cs(1)-O(3)#4	115.9(3)	O(13)-Cs(3)-O(16)#7	74.6(2)
O(7)-Cs(1)-O(3)#4	69.7(4)	O(14)#9-Cs(3)-O(16)#7	148.8(3)
O(6)#1-Cs(1)-O(3)#4	85.8(3)	O(1)-B(1)-O(3)#2	122.7(16)
O(7)#2-Cs(1)-O(3)#4	108.4(4)	O(1)-B(1)-O(2)	120.6(16)
O(2)#3-Cs(1)-O(3)#4	42.5(3)	O(3)#2-B(1)-O(2)	116.6(15)
O(4)#1-Cs(1)-O(3)#4	124.3(3)	O(4)-B(2)-O(3)	123.1(17)
O(6)-Cs(1)-O(8)#2	109.4(4)	O(4)-B(2)-O(2)	121.0(16)
O(7)-Cs(1)-O(8)#2	159.1(4)	O(3)-B(2)-O(2)	115.9(17)
O(6)#1-Cs(1)-O(8)#2	76.0(3)	O(4)-B(3)-O(6)	110.0(14)
O(7)#2-Cs(1)-O(8)#2	38.2(4)	O(4)-B(3)-O(5)	108.6(15)
O(2)#3-Cs(1)-O(8)#2	94.4(4)	O(6)-B(3)-O(5)	111.8(13)
O(4)#1-Cs(1)-O(8)#2	75.0(3)	O(4)-B(3)-O(1)#1	110.2(13)
O(3)#4-Cs(1)-O(8)#2	120.9(4)	O(6)-B(3)-O(1)#1	108.3(14)
O(6)-Cs(1)-O(1)#1	43.6(3)	O(5)-B(3)-O(1)#1	107.9(14)

O(7)-Cs(1)-O(1)#1	69.2(4)	O(5)-B(4)-O(10)	126.5(16)
O(6)#1-Cs(1)-O(1)#1	102.7(3)	O(5)-B(4)-O(11)	118.7(15)
O(7)#2-Cs(1)-O(1)#1	106.9(4)	O(10)-B(4)-O(11)	114.8(14)
O(2)#3-Cs(1)-O(1)#1	144.5(3)	O(6)-B(5)-O(11)	121.4(18)
O(4)#1-Cs(1)-O(1)#1	60.9(3)	O(6)-B(5)-O(12)	119.3(15)
O(3)#4-Cs(1)-O(1)#1	137.6(3)	O(11)-B(5)-O(12)	119.2(16)
O(8)#2-Cs(1)-O(1)#1	101.4(4)	O(13)-B(6)-O(12)	120.9(15)
O(15)#5-Cs(2)-O(8)#6	87.9(4)	O(13)-B(6)-O(16)	120.8(15)
O(15)#5-Cs(2)-O(13)	101.7(3)	O(12)-B(6)-O(16)	118.0(15)
O(8)#6-Cs(2)-O(13)	110.2(4)	O(15)-B(7)-O(14)	125.8(15)
O(15)#5-Cs(2)-O(7)	98.9(3)	O(15)-B(7)-O(16)	116.4(14)
O(8)#6-Cs(2)-O(7)	145.8(4)	O(14)-B(7)-O(16)	117.8(14)
O(13)-Cs(2)-O(7)	101.2(3)	O(14)-B(8)-O(15)#7	106.9(14)
O(15)#5-Cs(2)-O(14)#7	43.4(3)	O(14)-B(8)-O(13)	112.9(15)
O(8)#6-Cs(2)-O(14)#7	86.8(4)	O(15)#7-B(8)-O(13)	109.2(15)
O(13)-Cs(2)-O(14)#7	61.7(3)	O(14)-B(8)-O(10)#3	106.7(14)
O(7)-Cs(2)-O(14)#7	120.8(3)	O(15)#7-B(8)-O(10)#3	109.3(15)
O(15)#5-Cs(2)-O(9)	75.1(4)	O(13)-B(8)-O(10)#3	111.5(14)
O(8)#6-Cs(2)-O(9)	162.7(4)	O(7)-N(1)-O(8)	120.5(19)
O(13)-Cs(2)-O(9)	77.2(3)	O(7)-N(1)-O(9)	119.0(17)
O(7)-Cs(2)-O(9)	38.3(4)	O(8)-N(1)-O(9)	120.3(18)

Symmetry transformations used to generate equivalent atoms:

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

Table S4 The assignments of the Infrared absorption peaks for CBN.

Vibration mode description of characteristic absorption peak	Wavenumbers (cm^{-1})
B_3-O and N-O asymmetric stretching vibrations	1463, 1324
B_4-O asymmetric stretching vibrations	1253, 1083
B_3-O and N-O symmetric stretching vibrations	956, 902
B_4-O symmetric stretching vibrations	850, 833
B_3-O and N-O out-of-plane bending vibrations	761, 708
B_4-O and B_3-O bending vibrations	570, 534, 482

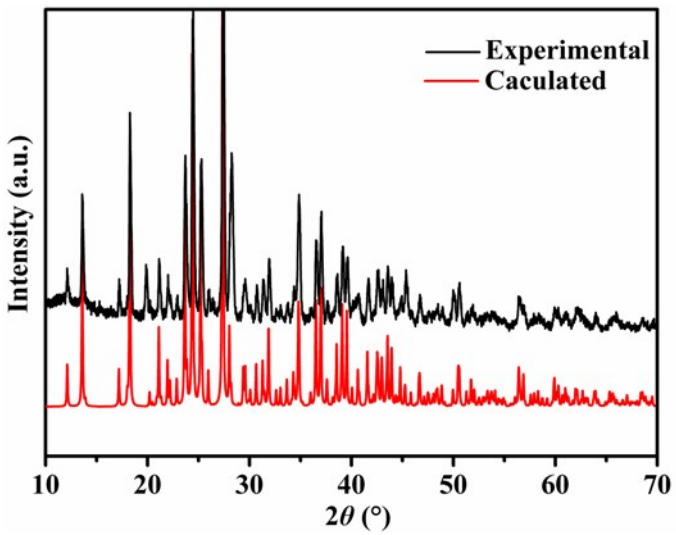

Figure S1 Comparison of calculated and experimental XRD patterns of CBN.

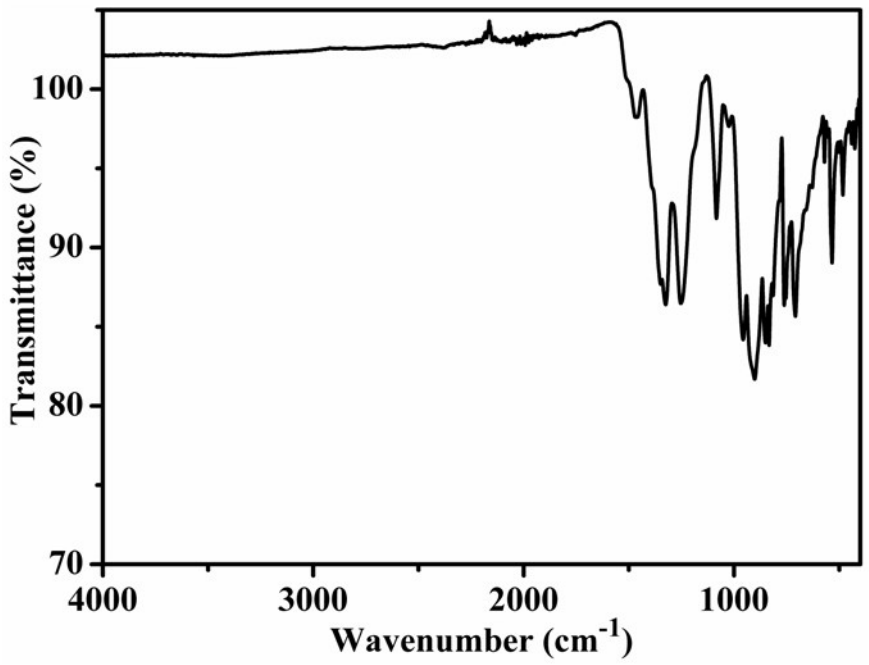

Figure S2 Infrared spectrum of CBN.

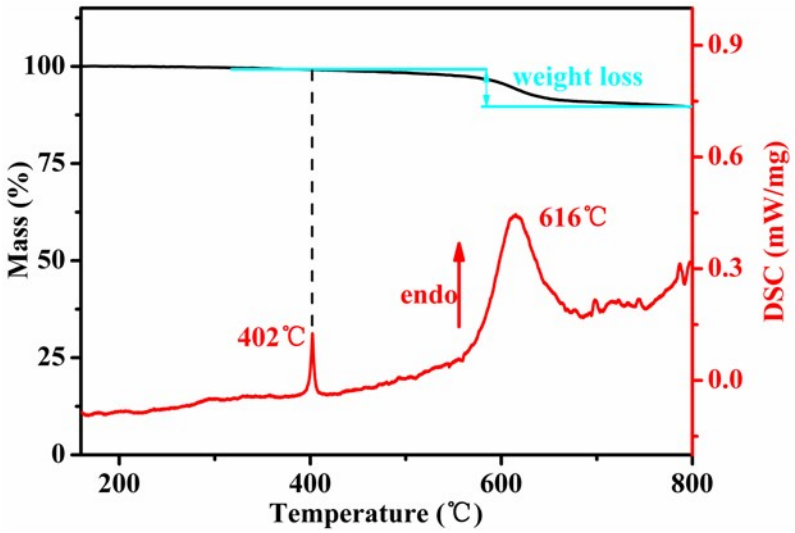

Figure S3 TG - DTA curves of CBN.

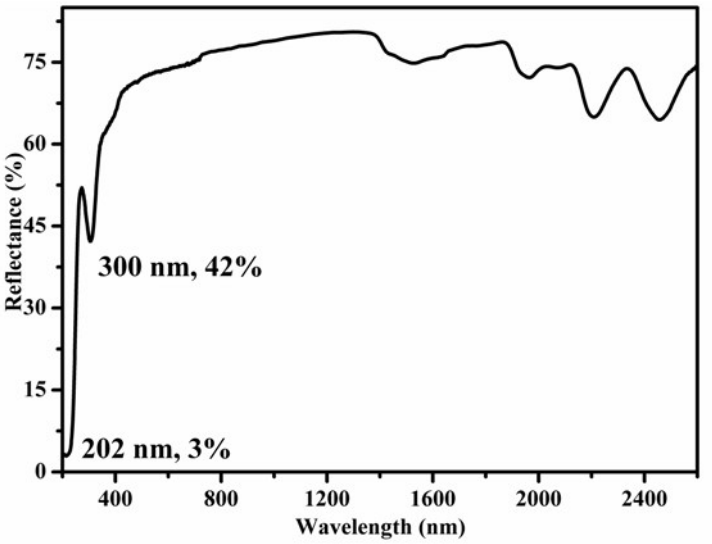

Figure S4. UV-vis-IR diffuse reflectance spectroscopy of CBN. The typical absorption band at 300 nm is similar to the spectrum of many other nitrates, such as $M_3B_6O_{10}NO_3$ (M = K, Rb), $K_2Ba(NO_3)_4$, $NaNO_3$, KNO_3, $RbNO_3$, and $CsNO_3$, etc.[6,16-17]

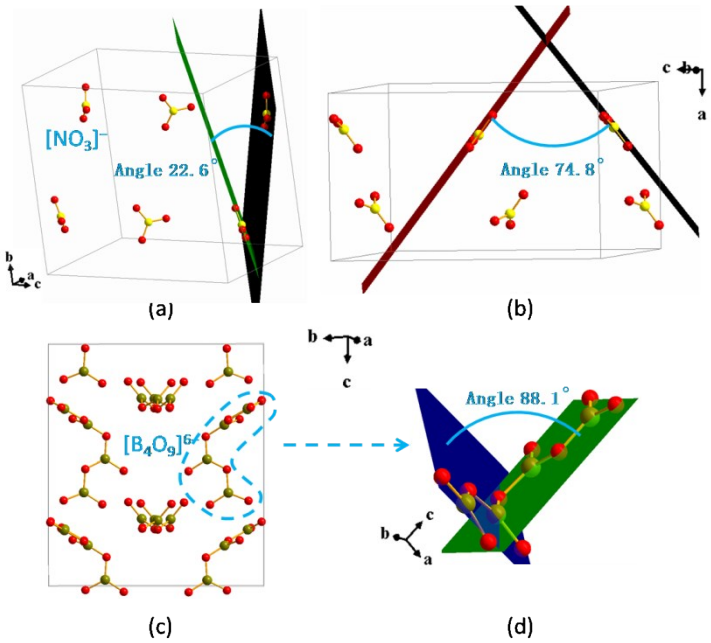

Figure S5. The arrangement of the NLO-active units of CBN. (a) The angle between the adjacent $[NO_3]^-$ plane in the direction of *b*-axis. (b) The angle between adjacent $[NO_3]^-$ planes in the direction of *c*-axis. (c) The linkage pattern of $[BO_3]^{3-}$ in a cell. Two $[BO_3]^{3-}$ units condense to a $[B_2O_5]^{4-}$ unit which further form a $[B_4O_9]^{6-}$ unit via sharing O atoms. (d) The $[B_4O_9]^{6-}$ unit formed by two almost perpendicular $[B_2O_5]^{4-}$ units.

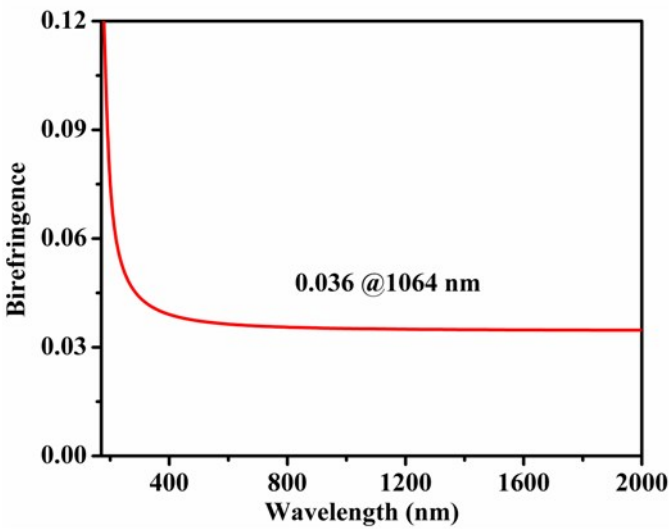

Figure S6. Calculated birefringence of CBN.

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