# Supporting Information

# Kyropoulos Growth and Characterization of Monoclinic α-$Bi_2B_8O_{15}$ Single Crystal with Noncentrosymmetric Structure

Mengdi Fan,[a] Guangda Wu,[a] Xinle Wang,[b] Fapeng Yu,[*,a] Chun Wang,[a] and Xian Zhao[*,a]

[a]Key Laboratory of Laser & Infrared System, Ministry of Education, State Key Laboratory of Crystal Materials, Shandong University, Qingdao, 266237, China

[b]Department of Physics and Electronic Science, Weifang University, Weifang, 261061, China

Corresponding authors: fapengyu@sdu.edu.cn (F. Yu); xianzhao@sdu.edu.cn (X. Zhao)

**Table S1** Crystallographic data for α-$Bi_2B_8O_{15}$ crystal.

| | |
|---|---|
| Phase Name | α-$Bi_2B_8O_{15}$ |
| R-Bragg | 2.285 |
| Space Group | $P2_1$ |
| Scale | $8.306\times10^{-5}$ |
| Cell Mass | 1488.880 |
| Cell Volume ($Å^3$) | 595.600 |
| Wt%-Rietveld | 100.000 |
| Double-Voigt\|Approach | |
| Crystal Size Lorentzian | 63.500 |
| k:1 L Vol-IB (nm) | 40.411 |
| k:0.89 L Vol-FWHM (nm) | 56.496 |
| Crystal Linear Absorption Coefficient. ($cm^{-1}$) | 562.114 |
| Crystal Density ($g/cm^3$) | 4.151 |
| Lattice Parameters | |
| *a* (Å) | 4.314 |
| *b* (Å) | 22.158 |
| *c* (Å) | 6.463 |
| *β* (°) | 105.407 |
| *α*=*γ* (°) | 90 |

**Table S2** Selected bond distances (Å) for α-$Bi_2B_8O_{15}$ crystal.

| Atoms | Symmetry | Distance(Å) | Atoms | Symmetry | Distance(Å) |
|---|---|---|---|---|---|
| Bi1 | x, y, z | - | O3 | x, y, z | 1.3516 |
| O6 | x, y, z | 2.2562 | O4 | x, y, z | 1.3413 |
| O4 | x, y, z | 2.7212 | B4 | x, y, z | - |
| O7 | x, y, z | 2.0917 | O4 | x, y, z | 1.5377 |
| O8 | x, y, z | 2.5219 | O5 | x, y, z | 1.4220 |
| O7 | 1+x, y, z | 2.6964 | O6 | x, y, z | 1.4877 |
| O11 | x, y, z | 2.1506 | O8 | x, y, z-1 | 1.4491 |
| Bi2 | x, y, z | - | B5 | x, y, z | - |
| O9 | x, y, z | 2.4904 | O5 | x, y, z | 1.3581 |
| O10 | 1+x, y, z | 2.7016 | O7 | x, y, z-1 | 1.3722 |
| O6 | x, y, z | 2.1182 | O8 | 1+x, y, z-1 | 1.3982 |
| O11 | x, y, z | 2.2933 | B6 | x, y, z | - |
| O13 | x, y, z | 2.8668 | O9 | x, y, 1+z | 1.4702 |
| O10 | x, y, z | 2.0843 | O11 | x, y, z | 1.4455 |
| B1 | x, y, z | - | O12 | x, y, z | 1.4674 |
| O1 | x, y, z | 1.4116 | O13 | x, y, z | 1.4968 |
| O2 | x, y, z | 1.3368 | B7 | x, y, z | - |
| O14 | 1-x, 1/2+y, 2-z | 1.3294 | O9 | x-1, y, 1+z | 1.3522 |
| B2 | x, y, z | - | O10 | x, y, 1+z | 1.3552 |
| O1 | x, y, z | 1.3908 | O12 | x, y, z | 1.3746 |
| O3 | x, y, z | 1.4462 | B8 | x, y, z | - |
| O15 | 1-x, 1/2+y, 1-z | 1.2441 | O13 | x, y, z | 1.3274 |
| B3 | x, y, z | - | O14 | x, y, z | 1.3751 |
| O2 | x, y, z | 1.3978 | O15 | x, y, z | 1.4038 |

**Table S3** Atomic coordinates for α-$Bi_2B_8O_{15}$ crystal.

| Atoms | Site | x/*a* | y/*b* | z/*c* | Occupied |
|---|---|---|---|---|---|
| Bi1 | 2a | 0.61092 | 0.78383 | 0.89404 | 1 |
| Bi2 | 2a | 0.82447 | 0.64754 | 0.66890 | 1 |
| B1 | 2a | 0.44200 | 0.98890 | 0.57100 | 1 |
| B2 | 2a | 0.46200 | 0.96440 | 0.20800 | 1 |
| B3 | 2a | 0.69300 | 0.89820 | 0.51100 | 1 |
| B4 | 2a | 0.86700 | 0.78630 | 0.48000 | 1 |
| B5 | 2a | 1.28000 | 0.78470 | 0.26500 | 1 |
| B6 | 2a | 0.57300 | 0.64470 | 1.08600 | 1 |
| B7 | 2a | 0.14700 | 0.64750 | 1.30400 | 1 |
| B8 | 2a | 0.60900 | 0.53210 | 1.08900 | 1 |
| O1 | 2a | 0.35700 | 1.00160 | 0.34900 | 1 |
| O2 | 2a | 0.60200 | 0.93870 | 0.65000 | 1 |
| O3 | 2a | 0.63200 | 0.91030 | 0.29900 | 1 |
| O4 | 2a | 0.82100 | 0.84540 | 0.59300 | 1 |
| O5 | 2a | 1.18000 | 0.78420 | 0.44730 | 1 |
| O6 | 2a | 0.83600 | 0.74290 | 0.64900 | 1 |
| O7 | 2a | 1.09800 | 0.79110 | 1.05700 | 1 |
| O8 | 2a | 0.61000 | 0.78130 | 1.28400 | 1 |
| O9 | 2a | 0.82900 | 0.65400 | 0.28500 | 1 |
| O10 | 2a | 0.33900 | 0.64100 | 0.50600 | 1 |
| O11 | 2a | 0.59500 | 0.68720 | 0.92080 | 1 |
| O12 | 2a | 0.25100 | 0.64880 | 1.12060 | 1 |
| O13 | 2a | 0.59700 | 0.58440 | 0.98700 | 1 |
| O14 | 2a | 0.64700 | 0.53020 | 1.30700 | 1 |
| O15 | 2a | 0.58000 | 0.47580 | 0.98600 | 1 |

**Table S4** Valence bonds calculation of α-$Bi_2B_8O_{15}$ crystal.

| $Bi(1)O_6$ octahedron | | $Bi(2)O_6$ octahedron | | $BO_3$ triangle | | |
|---|---|---|---|---|---|---|
| | $\nu_{ij}$ | | $\nu_{ij}$ | | $\nu_{ij}$ | $V_i$ |
| Bi(1)-O6 | 1.092 | Bi(2)-O4 | 0.157 | B(1)-O2 | 1.052 | |
| Bi(1)-O13 | 0.115 | Bi(2)-O11 | 0.990 | B(1)-O14 | 1.050 | 3.142 |
| Bi(1)-O9 | 0.326 | Bi(2)-O6 | 0.500 | B(1)-O1 | 1.041 | |
| Bi(1)-O11 | 0.544 | Bi(2)-O8 | 0.290 | B(2)-O15 | 1.055 | |
| Bi(1)-O10 | 1.082 | Bi(2)-O7 | 0.150 | B(2)-O1 | 1.052 | 3.155 |
| Bi(1)-O10 | 0.158 | Bi(2)-O7 | 1.083 | B(2)-O3 | 1.048 | |
| $V_i$ | 3.317 | $V_i$ | 3.170 | | | |

| $BO_x$ polyhedron | | | $BO_x$ polyhedron | | | $BO_3$ triangle | | |
|---|---|---|---|---|---|---|---|---|
| | $\nu_{ij}$ | $V_i$ | | $\nu_{ij}$ | $V_i$ | | $\nu_{ij}$ | $V_i$ |
| B(3)-O4 | 1.056 | | B(5)-O5 | 0.991 | | B(7)-O10 | 1.050 | |
| B(3)-O3 | 1.037 | 3.129 | B(5)-O7 | 0.984 | 2.947 | B(7)-O9 | 1.042 | 3.125 |
| B(3)-O2 | 1.035 | | B(5)-O8 | 0.971 | | B(7)-O12 | 1.034 | |
| B(4)-O4 | 0.771 | | B(6)-O9 | 0.748 | | B(8)-O13 | 1.082 | |
| B(4)-O6 | 0.780 | 3.111 | B(6)-O12 | 0.742 | 2.982 | B(8)-O14 | 1.076 | 3.225 |
| B(4)-O5 | 0.778 | | B(6)-O11 | 0.747 | | B(8)-O15 | 1.068 | |
| B(4)-O8 | 0.783 | | B(6)-O13 | 0.744 | | | | |

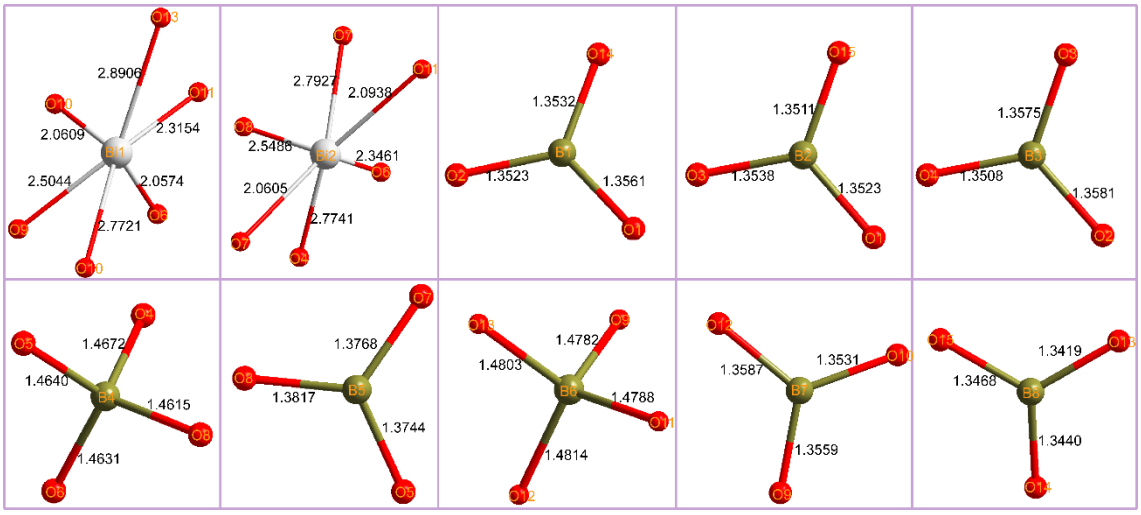


**Fig. S1** Coordination of Bi and B atoms with O in α-$Bi_2B_8O_{15}$ crystal.

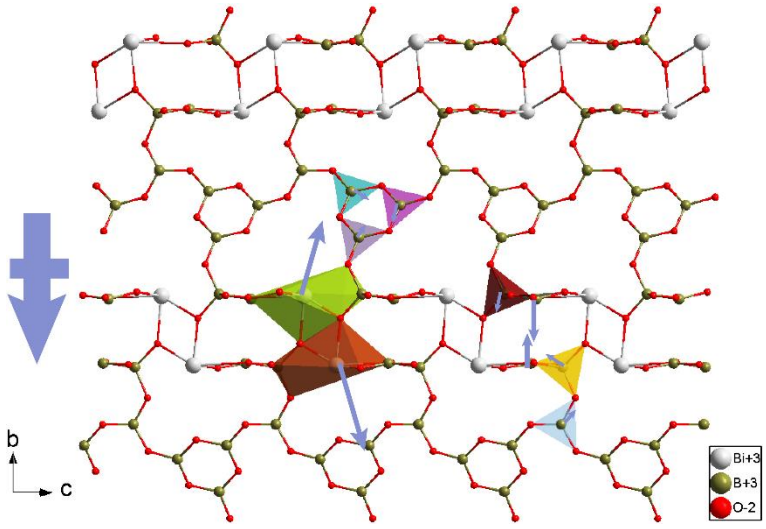


**Fig. S2** The directions of dipole moments for α-$Bi_2B_8O_{15}$ crystal.