Electronic Supporting Information

$LiCs_3AlB_7O_{14}$: Achieving the enhanced optical anisotropy via $[AlO_4]$ tetrahedra introduction to rearrange the anionic framework

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Experimental Section

Single crystal preparation. Single crystals of $LiCs_3AlB_7O_{14}$ were obtained *via* spontaneous crystallization from its melt with stoichiometric ratio since it is a congruently melting crystal. The raw materials and molar rate are as follow: $LiAlO_2$: Cs_2CO_3 : B_2O_3 = 1 : 1.5 : 3.5. The mixture was ground thoroughly and heated to 600 ℃ and held at 600 ℃ for 72 h. Then, they were cooled slowly to the room temperature at a rate of 3 °C h^{-1}. With this, the single crystals of $LiCs_3AlB_7O_{14}$ were obtained. The polycrystalline samples of $LiCs_3AlB_7O_{14}$ were obtained directly by grinding the as grown crystals.

Characterization. The powder XRD data of $LiCs_3AlB_7O_{14}$ were gathered by using the Cu Kαradiation (λ= 1.54056 Å) of the Bruker D2 PHASER X-ray diffractometer. The operating parameters of the instrument were scanned in the 2θ range from 5 to 70°with a scan rate of 1.2°min^{-1} and a scan step width of 0.02°. The single crystal structure of $LiCs_3AlB_7O_{14}$ was collected by using a Bruker D8 Venture single-crystal X-raydiffractometer with Mo-Kα radiation (λ = 0.71073 Å) at room temperature (25℃). Integration and absorption corrections of the collected data was completed by using SAINT and SCALE program, respectively.[1-2] The structure was solved by direct methods and then refined by full-matrix least squares on *F* with SHELXTL-14 program. PLATON was used to confirm the higher symmetry.[3] Infrared spectrum was carried out on a Shimadzu IR Affinity-1 Fourier transform S3 Infrared spectrometer. The sample is mixed with dried KBr (sample: KBr = 1 : 100), and the spectrum was collected in the range from 400 to 4000 cm^{-1} with a resolution of 2 cm^{-1}. The UV-Vis NIR diffuse reflectance spectrum was measured at room temperature with a Shimadzu SolidSpec-3700DUV spectrophotometer to determine the cutoff edge of $LiCs_3AlB_7O_{14}$. Thermal gravimetric (TG) analysis and differential scanning calorimetry (DSC) of $LiCs_3AlB_7O_{14}$ were carried out on a simultaneous NETZSCH STA 449C thermal analyzer instrument to evaluate the structural stability of $LiCs_3AlB_7O_{14}$. The measurement of the polycrystalline powders was put in Pt crucible and heated at a rate of 10 °C min^{-1} in the range of 40–800 °C under a flow of N_2.

Theoretical calculations. The first-principles calculations were performed by the plane-

wave pseudopotential method implemented in the CASTEP package.[4] The electronic structures, optical properties, and density of states (DOS) of $LiCs_3AlB_7O_{14}$ were calculated by the density functional theory (DFT) using the plane-wave pseudopotential in CASTEP. Meanwhile the generalized gradient approximation (GGA) of Perdew-Buker-Ernzerhof (PBE) was exerted. Interactions between ionic cores and electrons were described by the norm-conserving pseudop.[5]

Figure S1 (a) Dihedral angle α of $[B_2O_5]$ units in $[B_7O_{14}]$ units from $Li_4Cs_3B_7O_{14}$.[6] **(b) (c)** Dihedral angle α of $[B_2O_5]$ units in $[B_7O_{14}]$ units from $LiCs_3AlB_7O_{14}$.**(d-f)** The dihedral angles of Figures a-c are formed by B and O atoms.

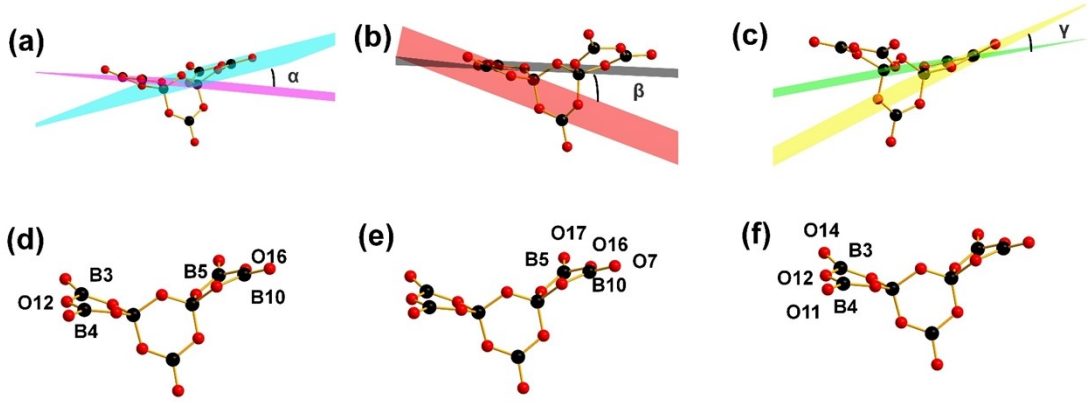

Figure S2 (a-c) Three dihedral angles of $[B_2O_5]$ units from α-$Li_4B_2O_5$.[7] **(d-f)** Three dihedral angles of $[B_2O_5]$ units from $LiAlB_2O_5$.[8]

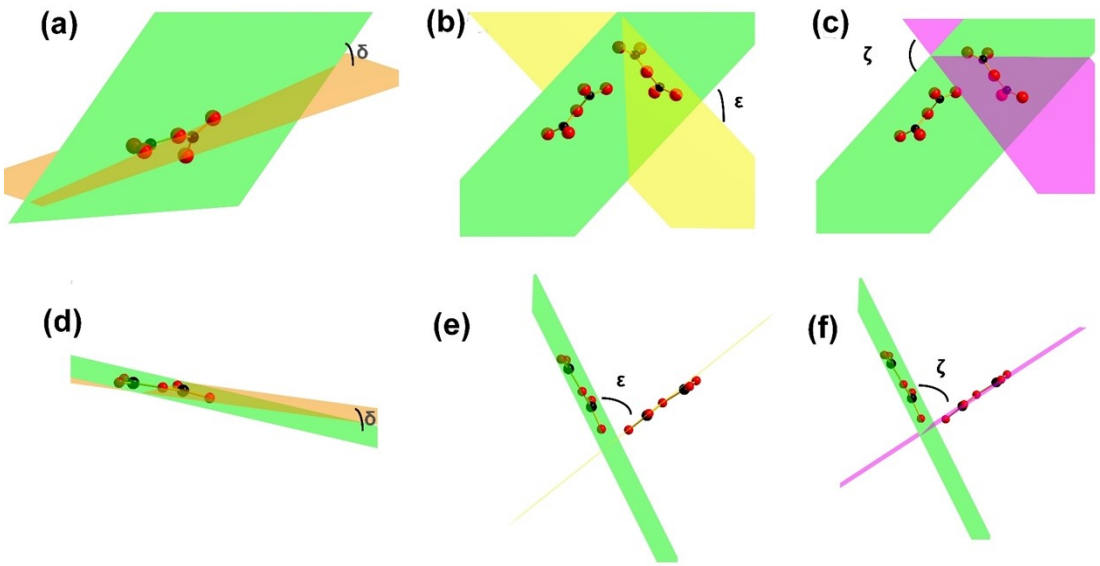

Figure S3. (a) Diagrammatic sketch of $[B_7O_{14}]$ units in optical indicatrix for $Li_4Cs_3B_7O_{14}$. **(b)** Diagrammatic sketch of $[B_7O_{14}]$ units in optical indicatrix for $LiCs_3AlB_7O_{14}$. **(c-d)** Arrangement of $[BO_3]$ units in Li_3BO_3 and $Li_3Al(BO_3)_2$.[9-10] **(e-f)** Arrangement of $[B_2O_5]$ units in α-$Li_4B_2O_5$ and $LiAlB_2O_5$.

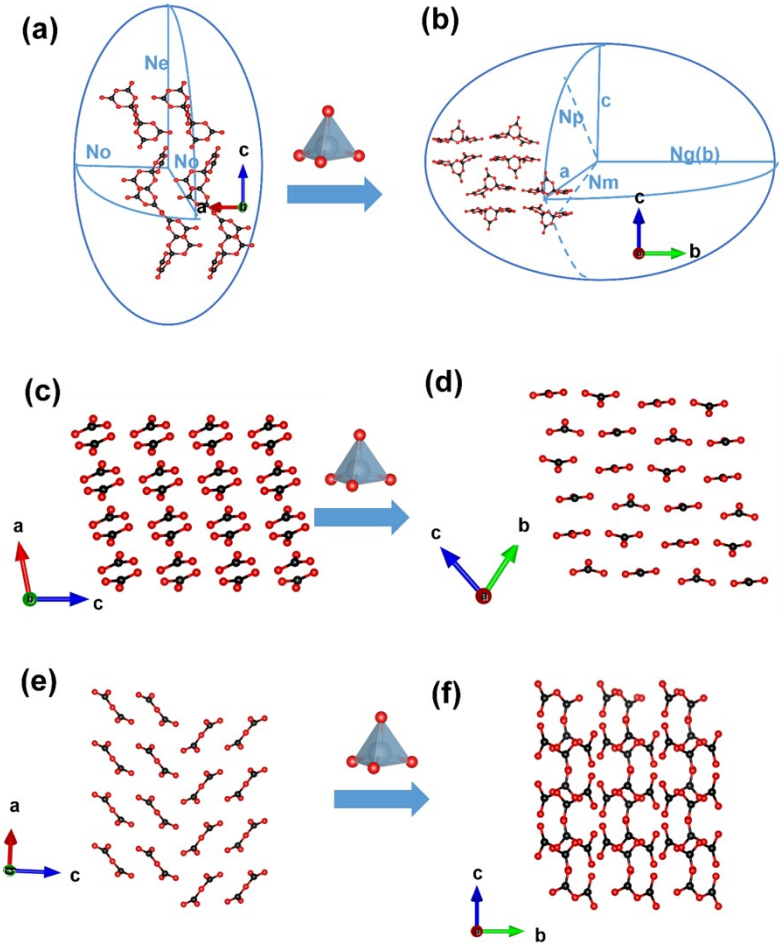

Figure S4. Band structure **(a)** and density of states **(b)** for $LiCs_3AlB_7O_{14}$.

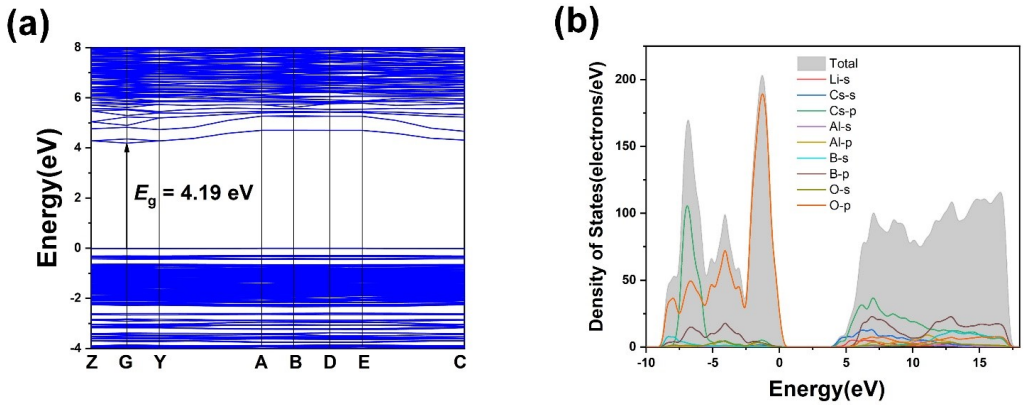

Table S1. Crystal data and structure refinement information.

Empirical formula	**$LiCs_3AlB_7O_{14}$**
Formula weight	732.32
Temperature/K	293(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	7.1302(3)
b/Å	21.6783(9)
c/Å	20.4145(9)
β/°	106.432(2)
Volume/Å^3	3026.6(2)
Z	8
ρ_{calc}g/cm^3	3.214
μ/mm^{-1}	7.314
F(000)	2624.0
Radiation	MoKα (λ = 0.71073)
2θrange for data collection/°	2.802 to 55.022
Completeness (%)	99.9
Index ranges	$-9 \le h \le 9$, $-28 \le k \le 28$, $-26 \le l \le 26$
Reflections collected	35129
Independent reflections	6956 [R_{int}= 0.0856, R_{sigma}= 0.0613]
Data/restraints/parameters	6956/0/500
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1= 0.0423, wR_2= 0.0733
Final R indexes [all data]	R_1= 0.0660, wR_2= 0.0872
Largest diff. peak/hole / e Å^{-3}	1.29/-1.10

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]^{1/2}$ 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 sum (BVS) calculations for $LiCs_3AlB_7O_{14}$.

Atom	*x*	*y*	*z*	*occ.*	*U*(eq)	BVS
Li(1)	3880(20)	9180(6)	1981(8)	1	32(3)	1.01
Li(2)	6130(20)	8615(10)	2964(8)	1	56(5)	0.87
Cs(1)	714.1(8)	7861.8(2)	2632.9(3)	1	27.98(14)	1.28
Cs(2)	4060.1(8)	8043.9(2)	4758.7(3)	1	30.29(14)	0.93
Cs(3)	9708.5(8)	8036.4(2)	633.1(3)	1	31.77(14)	0.79
Cs(4A)	6440(50)	5673(6)	2686(11)	0.3	59(2)	0.97
Cs(4B)	6800(6)	5685(3)	2757(3)	0.7	32.7(9)	
Cs(5A)	7330(20)	5262(12)	4609(8)	0.34	73(3)	0.89
Cs(5B)	7199(7)	5173(2)	4651(2)	0.66	35.7(14)	
Cs(6A)	3432(15)	9719(8)	5834(3)	0.18	31(3)	0.83
Cs(6B)	3351(5)	9823(3)	5817.4(17)	0.82	71.4(12)	
Al(1)	9968(3)	6261.9(10)	1433.8(12)	1	21.2(5)	3.02
Al(2)	7126(3)	1359.3(10)	1112.6(12)	1	19.8(5)	2.93
B(1)	9942(12)	3999(4)	1185(5)	1	19.9(18)	3.04
B(2)	1588(12)	3002(4)	990(5)	1	19.6(17)	3.07
B(3)	7387(13)	4274(4)	1790(5)	1	26(2)	3.01
B(4)	9979(13)	5010(4)	1747(4)	1	20.6(17)	3.11
B(5)	791(12)	1914(4)	1185(5)	1	22.4(18)	3.10
B(6)	7270(12)	126(4)	1571(4)	1	20.4(17)	3.03
B(7)	9911(13)	9430(4)	1472(5)	1	24.1(19)	3.03
B(8)	326(13)	3728(4)	39(5)	1	24.3(19)	3.09
B(9)	6781(12)	9023(4)	1524(5)	1	20.7(18)	2.98
B(10)	4189(12)	2173(4)	1305(4)	1	20.4(17)	3.07
B(11)	4599(13)	8616(4)	419(5)	1	24.8(19)	3.14
B(12)	3273(13)	7092(4)	1701(5)	1	27(2)	3.10
B(13)	6430(13)	6908(4)	1518(5)	1	24.6(19)	3.13
B(14)	5176(10)	7989(3)	1480(4)	1	10.0(14)	2.89
O(1)	1350(7)	3498(2)	1423(2)	1	18.7(11)	2.11
O(2)	8105(7)	3889(2)	1376(3)	1	22.0(11)	2.12
O(3)	6464(7)	695(2)	1482(3)	1	23.4(11)	2.05
O(4)	234(7)	2486(2)	989(3)	1	23.2(11)	2.10
O(5)	8983(7)	22(2)	1398(3)	1	25.4(12)	1.87
O(6)	5890(7)	8560(2)	1849(2)	1	17.9(10)	1.93
O(7)	6018(7)	2001(2)	1357(3)	1	32.3(14)	2.07
O(8)	9404(8)	4048(2)	431(3)	1	31.2(13)	2.00
O(9)	4194(7)	8096(2)	738(3)	1	27.3(12)	1.98
O(10)	4598(7)	6693(2)	1539(3)	1	30.1(13)	1.98
O(11)	690(8)	5582(2)	1862(3)	1	28.4(12)	1.95
O(12)	8207(8)	4871(2)	1878(3)	1	36.3(15)	2.10

O(13)	6778(7)	7523(2)	1530(3)	1	26.2(12)	1.96
O(14)	6009(8)	4122(3)	2076(3)	1	31.2(13)	1.79
O(15)	1532(8)	6877(2)	1715(3)	1	39.8(16)	2.13
O(16)	2714(7)	1734(2)	1228(3)	1	32.1(14)	2.03
O(17)	9635(7)	1472(2)	1325(3)	1	28.5(13)	1.91
O(18)	1382(8)	3196(2)	291(3)	1	29.4(13)	1.94
O(19)	97(11)	3905(3)	9399(3)	1	51.5(18)	2.05
O(20)	7694(8)	6472(3)	1491(4)	1	43.6(17)	2.00
O(21)	3715(11)	8717(3)	9758(3)	1	58(2)	1.87
O(22)	3658(7)	7705(2)	1764(3)	1	24.8(12)	2.03
O(23)	885(8)	4567(2)	1490(3)	1	32.3(14)	2.17
O(24)	3666(7)	2780(2)	1294(3)	1	27.9(13)	1.95
O(25)	8914(7)	8957(2)	1671(3)	1	21.6(11)	2.07
O(26)	1557(7)	9371(2)	1314(3)	1	26.2(12)	1.85
O(27)	6294(7)	9648(2)	1764(3)	1	22.4(11)	1.87
O(28)	5946(8)	9028(2)	767(3)	1	30.0(13)	1.95

Table S3. Anisotropic displacement parameters ($Å^2×10^3$) for $LiCs_3AlB_7O_{14}$.

Atom	*U*11	*U*22	*U*33	*U*23	*U*13	*U*12
Li(1)	30(7)	26(7)	43(9)	6(6)	17(7)	12(6)
Li(2)	29(8)	105(15)	31(9)	-5(9)	3(7)	26(9)
Cs(1)	34.7(3)	24.0(3)	28.3(3)	-2.8(2)	14.0(2)	2.5(2)
Cs(2)	33.3(3)	28.0(3)	31.6(3)	2.7(2)	12.4(2)	6.7(2)
Cs(3)	31.1(3)	30.9(3)	33.5(3)	-5.0(2)	9.4(2)	4.1(2)
Cs(4A)	110(7)	23(2)	71(6)	3(3)	72(5)	7(4)
Cs(4B)	42(2)	25.1(9)	35.8(14)	-5.6(7)	19.2(18)	2.0(5)
Cs(5A)	52(4)	95(5)	57(4)	-23(3)	-9(3)	42(3)
Cs(5B)	32.7(12)	40(2)	33.9(13)	-12.7(7)	8.0(10)	5.9(14)
Cs(6A)	33(4)	36(4)	28(6)	-4(4)	15(4)	-15(2)
Cs(6B)	61.1(13)	58.5(13)	118(3)	-45.4(14)	63.2(17)	-26.8(8)
Al(1)	25.0(11)	13.4(10)	29.6(13)	1.6(9)	15.0(10)	1.1(9)
Al(2)	17.7(10)	14.7(10)	27.4(12)	1.9(9)	6.9(9)	-2.1(9)
B(1)	22(4)	9(4)	33(5)	-8(3)	15(4)	-2(3)
B(2)	18(4)	10(4)	31(5)	-2(3)	7(4)	1(3)
B(3)	25(4)	19(4)	38(5)	7(4)	17(4)	2(4)
B(4)	30(5)	13(4)	23(4)	-1(3)	14(4)	-1(3)
B(5)	20(4)	22(4)	26(5)	3(4)	8(4)	5(4)
B(6)	21(4)	17(4)	25(5)	0(3)	10(4)	2(3)
B(7)	24(4)	21(4)	29(5)	7(4)	10(4)	4(4)
B(8)	31(5)	16(4)	27(5)	-1(4)	9(4)	-1(4)
B(9)	21(4)	13(4)	33(5)	-1(4)	16(4)	-5(3)
B(10)	19(4)	21(4)	21(4)	-1(3)	6(3)	-4(3)
B(11)	24(4)	28(5)	21(5)	-1(4)	4(4)	-3(4)
B(12)	27(5)	19(4)	41(6)	-8(4)	21(4)	-5(4)
B(13)	22(4)	29(5)	24(5)	-1(4)	7(4)	0(4)
B(14)	8(3)	9(3)	14(4)	3(3)	5(3)	3(3)
O(1)	24(3)	13(2)	21(3)	-2(2)	10(2)	4(2)
O(2)	22(3)	19(3)	28(3)	-7(2)	11(2)	-2(2)
O(3)	23(3)	12(2)	36(3)	3(2)	9(2)	2(2)
O(4)	19(2)	14(2)	38(3)	1(2)	9(2)	4(2)
O(5)	25(3)	14(2)	42(3)	9(2)	18(3)	4(2)
O(6)	19(2)	15(2)	25(3)	4(2)	14(2)	-1(2)
O(7)	17(3)	20(3)	63(4)	3(3)	17(3)	2(2)
O(8)	38(3)	30(3)	27(3)	8(2)	11(3)	11(3)
O(9)	28(3)	18(3)	32(3)	-3(2)	4(2)	-2(2)
O(10)	25(3)	11(2)	61(4)	-5(3)	24(3)	0(2)
O(11)	35(3)	17(3)	33(3)	-2(2)	10(3)	-5(2)
O(12)	35(3)	23(3)	63(4)	-12(3)	34(3)	-2(3)
O(13)	19(3)	18(3)	48(4)	0(2)	20(3)	0(2)
O(14)	27(3)	33(3)	41(4)	-3(3)	21(3)	-7(2)

O(15)	29(3)	23(3)	80(5)	-9(3)	37(3)	-10(3)
O(16)	18(3)	14(3)	70(4)	6(3)	21(3)	1(2)
O(17)	16(3)	17(3)	55(4)	8(3)	13(3)	1(2)
O(18)	45(3)	20(3)	30(3)	-3(2)	21(3)	6(3)
O(19)	81(5)	48(4)	31(4)	9(3)	26(4)	17(4)
O(20)	27(3)	24(3)	85(5)	-5(3)	25(3)	3(3)
O(21)	69(5)	70(5)	28(4)	6(3)	2(3)	-19(4)
O(22)	22(3)	11(2)	48(4)	-2(2)	20(3)	-2(2)
O(23)	29(3)	25(3)	49(4)	-11(3)	22(3)	-7(2)
O(24)	21(3)	13(2)	53(4)	5(2)	15(3)	3(2)
O(25)	20(3)	16(2)	31(3)	2(2)	11(2)	3(2)
O(26)	20(3)	28(3)	34(3)	7(2)	13(2)	5(2)
O(27)	23(3)	11(2)	39(3)	2(2)	19(2)	0(2)
O(28)	33(3)	31(3)	25(3)	6(2)	7(3)	-15(3)

Table S4. Bond lengths (Å) and angles (°) for $LiCs_3AlB_7O_{14}$.

Al(1)-O(11)	1.716(6)	O(11)-Al(1)-O(15)	114.9(3)
Al(1)-O(15)	1.730(6)	O(11)-Al(1)-O(19)	104.0(3)
Al(1)-O(19)	1.727(6)	O(11)-Al(1)-O(20)	110.2(3)
Al(1)-O(20)	1.719(6)	O(19)-Al(1)-O(15)	108.9(3)
Al(2)-O(3)	1.752(5)	O(20)-Al(1)-O(15)	107.8(3)
Al(2)-O(7)	1.741(6)	O(20)-Al(1)-O(19)	111.0(4)
Al(2)-O(17)	1.735(5)	O(7)-Al(2)-O(3)	109.5(3)
Al(2)-O(21)	1.717(7)	O(17)-Al(2)-O(3)	113.1(3)
B(1)-O(1)	1.464(9)	O(17)-Al(2)-O(7)	109.6(3)
B(1)-O(2)	1.488(9)	O(21)-Al(2)-O(3)	108.0(3)
B(1)-O(8)	1.480(10)	O(21)-Al(2)-O(7)	108.7(4)
B(1)-O(23)	1.456(9)	O(21)-Al(2)-O(17)	107.8(3)
B(2)-O(1)	1.432(9)	O(1)-B(1)-O(2)	111.5(6)
B(2)-O(4)	1.476(9)	O(1)-B(1)-O(8)	110.5(6)
B(2)-O(18)	1.456(10)	O(8)-B(1)-O(2)	107.1(6)
B(2)-O(24)	1.514(9)	O(23)-B(1)-O(1)	107.1(6)
B(3)-O(2)	1.386(10)	O(23)-B(1)-O(2)	110.9(6)
B(3)-O(12)	1.410(10)	O(23)-B(1)-O(8)	109.6(6)
B(3)-O(14)	1.319(9)	O(1)-B(2)-O(4)	112.2(6)
B(4)-O(11)	1.335(9)	O(1)-B(2)-O(18)	113.0(6)
B(4)-O(12)	1.397(9)	O(1)-B(2)-O(24)	105.0(6)
B(4)-O(23)	1.343(9)	O(4)-B(2)-O(24)	108.9(6)
B(5)-O(4)	1.330(9)	O(18)-B(2)-O(4)	109.5(6)
B(5)-O(16)	1.403(9)	O(18)-B(2)-O(24)	108.0(6)
B(5)-O(17)	1.347(10)	O(2)-B(3)-O(12)	114.7(6)
B(6)-O(3)	1.351(9)	O(14)-B(3)-O(2)	124.8(7)
B(6)-O(5)	1.383(9)	O(14)-B(3)-O(12)	120.5(7)
B(6)-O(27)	1.368(9)	O(11)-B(4)-O(12)	119.1(7)
B(7)-O(5)	1.432(9)	O(11)-B(4)-O(23)	122.1(7)
B(7)-O(25)	1.374(9)	O(23)-B(4)-O(12)	118.7(7)
B(7)-O(26)	1.307(9)	O(4)-B(5)-O(16)	118.8(7)
B(8)-O(8)	1.362(10)	O(4)-B(5)-O(17)	125.4(7)
B(8)-O(18)	1.393(10)	O(17)-B(5)-O(16)	115.8(7)
B(8)-O(19)	1.325(10)	O(3)-B(6)-O(5)	119.3(7)
B(9)-O(6)	1.446(9)	O(3)-B(6)-O(27)	119.9(6)
B(9)-O(25)	1.472(9)	O(27)-B(6)-O(5)	120.5(7)
B(9)-O(27)	1.514(9)	O(25)-B(7)-O(5)	115.9(6)
B(9)-O(28)	1.490(10)	O(26)-B(7)-O(5)	118.8(7)
B(10)-O(7)	1.332(9)	O(26)-B(7)-O(25)	125.1(7)
B(10)-O(16)	1.394(9)	O(8)-B(8)-O(18)	120.3(7)
B(10)-O(24)	1.365(10)	O(19)-B(8)-O(8)	119.1(7)
B(11)-O(9)	1.371(10)	O(19)-B(8)-O(18)	120.4(7)
B(11)-O(21)	1.336(11)	O(6)-B(9)-O(25)	113.7(6)

B(11)-O(28)	1.356(10)	O(6)-B(9)-O(27)	107.6(6)
B(12)-O(10)	1.388(9)	O(6)-B(9)-O(28)	112.5(6)
B(12)-O(15)	1.333(10)	O(25)-B(9)-O(27)	109.8(6)
B(12)-O(22)	1.356(9)	O(25)-B(9)-O(28)	107.4(6)
B(13)-O(10)	1.398(10)	O(28)-B(9)-O(27)	105.6(6)
B(13)-O(13)	1.355(10)	O(7)-B(10)-O(16)	120.5(7)
B(13)-O(20)	1.318(10)	O(7)-B(10)-O(24)	121.9(7)
B(14)-O(6)	1.463(8)	O(24)-B(10)-O(16)	117.5(7)
B(14)-O(9)	1.496(9)	O(21)-B(11)-O(9)	120.8(8)
B(14)-O(13)	1.507(8)	O(21)-B(11)-O(28)	118.8(8)
B(14)-O(22)	1.498(8)	O(28)-B(11)-O(9)	120.4(7)
O(6)-B(14)-O(9)	112.7(5)	O(15)-B(12)-O(10)	119.3(7)
O(6)-B(14)-O(13)	112.6(5)	O(15)-B(12)-O(22)	120.3(7)
O(6)-B(14)-O(22)	109.4(5)	O(22)-B(12)-O(10)	120.0(7)
O(9)-B(14)-O(13)	107.5(5)	O(13)-B(13)-O(10)	119.7(7)
O(9)-B(14)-O(22)	105.9(5)	O(20)-B(13)-O(10)	114.7(7)
O(22)-B(14)-O(13)	108.4(5)	O(20)-B(13)-O(13)	125.6(7)

Symmetry transformations used to generate equivalent atoms:

#1 -1+X,+Y,+Z	#2 1-X,1/2+Y,1/2-Z	#3 -X,1/2+Y,1/2-Z
#4 2-X,2-Y,1-Z	#5 1+X,+Y,+Z	#6 2-X,1/2+Y,1/2-Z
#7 1+X,3/2-Y,1/2+Z	#8 2+X,3/2-Y,1/2+Z	#9 1-X,1-Y,-Z
#10 1-X,-1/2+Y,1/2-Z	#11 2-X,-1/2+Y,1/2-Z	#12 +X,3/2-Y,1/2+Z
#13 -1+X,3/2-Y,-1/2+Z	#14 -X,1-Y,-Z	#15 -X,-1/2+Y,1/2-Z
#16 -1+X,-1+Y,+Z	#17 -2+X,3/2-Y,-1/2+Z	#18 +X,3/2-Y,-1/2+Z
#19 1+X,1+Y,+Z		

Table S5. The three dihedral angles formed by two $[B_2O_5]$ units within the $[B_7O_{14}]$.

Compound	B-O isolated units	Dihedral Angle	Plane	Reference
		α	B3,O12,B4	
			B5,O16,B10	
	$[B_7O_{14}]$-1	β	O7,B10,O16	
			O16,B5,O17	
		γ	O11,B4,O12	
$LiCs_3AlB_7O_{14}$			O14,B3,O12	
		α	B6,O5,B7	this work
			B12,O10,B13	
	$[B_7O_{14}]$-2	β	O3,B6,O5	
			O5,B7,O26	
		γ	O15,B12,O10	
			O20,B13,O10	
		α	B1,B2,O7	
			B1,B2,O7	
$Li_4Cs_3B_7O_{14}$	$[B_7O_{14}]$	β	O2,B1,O7	6
			O6,B2,O7	
		γ	O2,B1,O7	
			O6,B2,O7	

References and Notes

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