Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

$Pb_2Bi_2GaB_3O_{11}$, A New Congruent-Melting Galloborate Containing Two Types of Asymmetric Cations with a Moderate Birefringence

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Table S1 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Pb_2Bi_2GaB_3O_{11}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	X	Y	Z	U(eq)
Bi(1)	4338(1)	2993(1)	-68(1)	13(1)
Pb(1)	1576(1)	5926(1)	599(1)	17(1)
Ga(1)	2500	2500	0	9(1)
B(1)	0	5170(20)	2500	5(4)
B(2)	3249(9)	5078(19)	2390(30)	8(3)
O(1)	644(7)	4390(13)	1941(18)	18(3)
O(2)	1798(7)	1524(12)	1876(17)	13(2)
O(3)	2587(7)	4369(13)	1777(18)	15(2)
O(4)	3966(7)	4466(13)	2323(19)	21(3)
O(5)	5000	1710(20)	2500	30(5)
O(6)	3419(6)	1552(12)	995(16)	9(2)

Table S2 Bond lengths [Å] and angles [deg] for $Pb_2Bi_2GaB_3O_{11}$.

Bi(1)-O(6)	2.167(10)	O(2)#1-Bi(1)-O(1)#1	84.2(4)
Bi(1)-O(4)	2.181(13)	O(5)-Bi(1)-O(1)#1	87.8(5)
Bi(1)-O(2)#1	2.354(12)	O(1)-Pb(1)-O(3)	92.3(4)
Bi(1)-O(5)	2.370(9)	O(1)-Pb(1)-O(6)#2	75.8(4)
Bi(1)-O(1)#1	2.466(12)	O(3)-Pb(1)-O(6)#2	79.0(4)
Pb(1)-O(1)	2.302(12)	O(1)-Pb(1)-O(6)#1	69.3(4)
Pb(1)-O(3)	2.367(12)	O(3)-Pb(1)-O(6)#1	67.7(4)
Pb(1)-O(6)#2	2.375(11)	O(6)#2-Pb(1)-O(6)#1	129.7(3)
Pb(1)-O(6)#1	2.449(10)	O(6)-Ga(1)-O(6)#1	180.0(3)
Ga(1)-O(6)	1.920(11)	O(6)-Ga(1)-O(2)	95.4(5)
Ga(1)-O(6)#1	1.920(11)	O(6)#1-Ga(1)-O(2)	84.6(5)
Ga(1)-O(2)	1.964(11)	O(6)-Ga(1)-O(2)#1	84.6(5)
Ga(1)-O(2)#1	1.964(11)	O(6)#1-Ga(1)-O(2)#1	95.4(5)
Ga(1)-O(3)#1	2.054(12)	O(2)-Ga(1)-O(2)#1	180.0(8)
Ga(1)-O(3)	2.054(12)	O(6)-Ga(1)-O(3)#1	84.9(5)
B(1)-O(1)#3	1.368(16)	O(6)#1-Ga(1)-O(3)#1	95.1(5)
B(1)-O(1)	1.368(16)	O(2)-Ga(1)-O(3)#1	88.9(5)
B(1)-O(5)#4	1.37(3)	O(2)#1-Ga(1)-O(3)#1	91.1(5)
B(2)-O(4)	1.36(2)	O(6)-Ga(1)-O(3)	95.1(5)
B(2)-O(3)	1.370(19)	O(6)#1-Ga(1)-O(3)	84.9(5)
B(2)-O(2)#2	1.379(19)	O(2)-Ga(1)-O(3)	91.1(5)
O(6)-Bi(1)-O(4)	83.5(4)	O(2)#1-Ga(1)-O(3)	88.9(5)
O(6)-Bi(1)-O(2)#1	70.5(4)	O(3)#1-Ga(1)-O(3)	180.0(7)
O(4)-Bi(1)-O(2)#1	91.7(4)	O(1)#3-B(1)-O(1)	119.2(19)
O(6)-Bi(1)-O(5)	80.0(4)	O(1)#3-B(1)-O(5)#4	120.4(9)
O(4)-Bi(1)-O(5)	83.4(4)	O(1)-B(1)-O(5)#4	120.4(9)
O(2)#1-Bi(1)-O(5)	150.5(3)	O(4)-B(2)-O(3)	124.9(14)
O(6)-Bi(1)-O(1)#1	71.1(4)	O(4)-B(2)-O(2)#2	116.1(13)
O(4)-Bi(1)-O(1)#1	154.2(4)	O(3)-B(2)-O(2)#2	119.0(13)

Symmetry transformations used to generate equivalent atoms:

#1	-x+1/2,-y+1/2,-z	#2	-x+1/2,y+1/2,-z+1/2
#3	-x,y,-z+1/2	#4	x-1/2,y+1/2,z
#5	-x+1/2,y-1/2,-z+1/2	#6	x+1/2,y-1/2,z
#7	-x+1,y,-z+1/2		

Table S3 The calculated anisotropic polarizability of BO_3, PbO_5, BiO_6.

Groups	BO_3	PbO_5	BiO_6
$\Delta\alpha$ (a.u.)	8.6	48.3	44.7

Figure S1 The unit cell and asymmetric unit of $Pb_2Bi_2GaB_3O_{11}$.

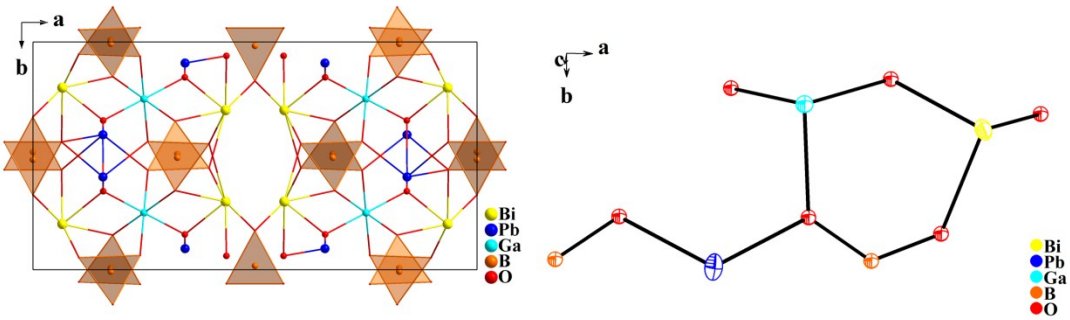

Figure S2 The coordination environments of cations in $Pb_2Bi_2GaB_3O_{11}$.

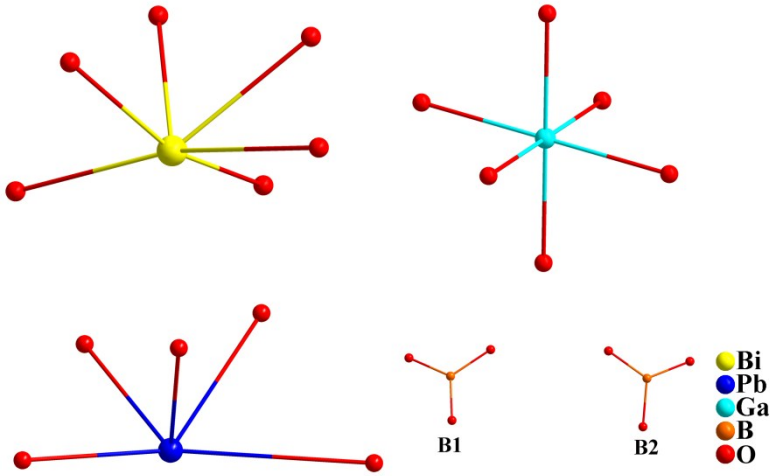

Figure S3 The BO_3 groups in $Pb_2Bi_2GaB_3O_{11}$.

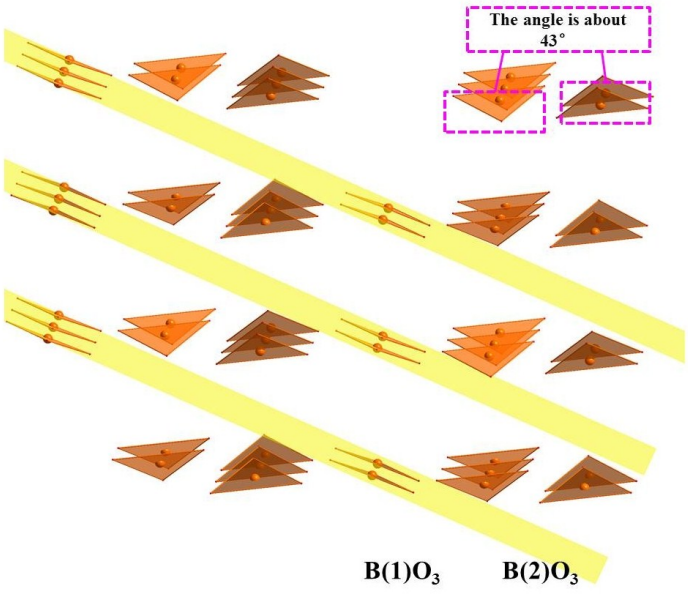

Figure S4 The UV-Vis-NIR diffuse reflectance spectrum (a) and IR spectrum (b).

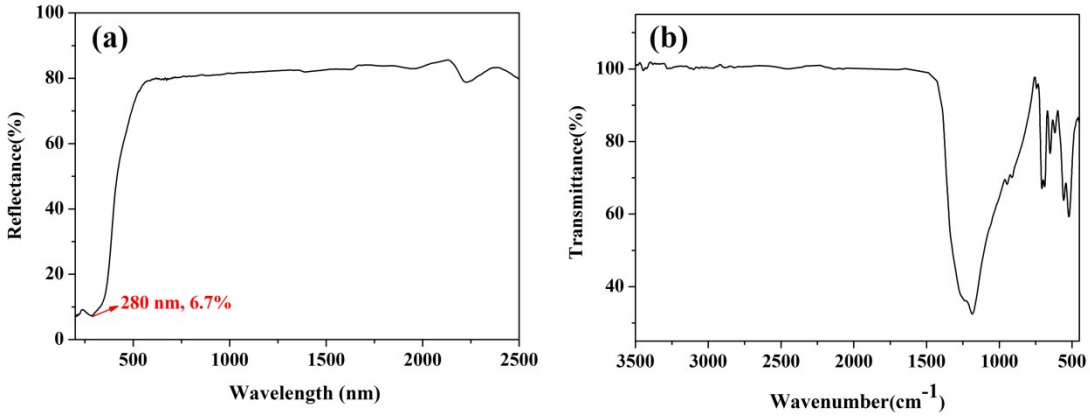

Figure S5 TG-DSC curves of $Pb_2Bi_2GaB_3O_{11}$.