Electronic Supporting Information

$Ba_{2.5}Pb_{1.5}B_{12}O_{22}$: Structural Transformation from Centrosymmetric to Noncentrosymmetric Space Group via Introducing Pb into $Ba_2B_6O_{11}$

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Table S1. Atomic coordinates, equivalent isotropic displacement parameters ($Å^2 \times 10^3$), and BVS for $Ba_{2.5}Pb_{1.5}B_{12}O_{22}$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x	y	z	U(eq)	BVS
Ba1B	0	-0.84081(6)	-0.7288(5)	0.03072(19)	2.29
Pb1B	0	-0.84081(6)	-0.7288(5)	0.03072(19)	2.29
Pb2B	-0.01384(4)	-0.58705(7)	-0.3736(5)	0.0245(3)	2.24
Ba2	-0.17856(3)	-0.74365(5)	-0.1025(5)	0.01751(14)	2.27
B1	-0.1852(5)	-0.5348(9)	-0.4433(13)	0.0155(13)	3.09
B2	-0.1659(5)	-0.4002(9)	-0.2086(13)	0.0146(17)	3.06
B3	-0.1471(5)	-0.7541(9)	-0.4972(13)	0.0141(15)	3.12
B4	-0.3118(5)	-0.4696(10)	-0.4218(13)	0.0192(19)	3.00
B5	-0.0649(6)	-0.9188(10)	-0.3997(13)	0.0203(19)	3.07
B6	0	-0.6542(9)	-0.0036(10)	0.029(3)	3.14
B7	0.0172(3)	-0.8397(6)	-0.1691(4)	0.017(4)	2.98
O1	-0.1614(3)	-0.4215(5)	-0.3646(9)	0.0140(11)	2.10
O2	-0.1665(4)	-0.2789(6)	-0.1546(9)	0.0167(13)	1.93
O3	-0.2016(3)	-0.8445(6)	-0.4386(9)	0.0162(12)	2.01
O4A	-0.3804(5)	-0.4989(15)	-0.3775(19)	0.015(3)	2.16
O4B	-0.3787(5)	-0.5208(14)	-0.4394(18)	0.014(3)	1.63
O5	-0.1464(3)	-0.6443(5)	-0.3958(8)	0.0160(11)	2.10
O6	-0.1750(4)	-0.5045(6)	-0.6090(10)	0.0306(14)	2.19
O7	0	-0.9762(8)	-0.4443(11)	0.0140(16)	2.24
O8	-0.2612(3)	-0.5570(6)	-0.4195(9)	0.0232(13)	2.01
O9	-0.0793(3)	-0.8121(6)	-0.4968(9)	0.0166(11)	2.20
O10	0	-0.3727(11)	-0.3499(13)	0.036(3)	2.15
O11	0.0726(6)	-0.9029(12)	-0.2340(12)	0.023(3)	2.13
O12	0.0276(5)	-0.7668(10)	-0.0398(11)	0.022(2)	2.04
O13	-0.0486(5)	-0.8492(11)	-0.2334(12)	0.015(2)	1.64
O14	0.0325(9)	-0.5813(13)	-0.1099(19)	0.044(4)	1.96

Table S2. Selected bond lengths (Å) and angles (deg.) for $Ba_{2.5}Pb_{1.5}B_{12}O_{22}$.

Ba(1B)-O(10)#1	2.517(13)	B(2)-O(1)	1.365(12)
Ba(1B)-O(9)	2.524(6)	B(2)-O(2)	1.382(11)
Ba(1B)-O(9)#2	2.524(6)	B(3)-O(9)	1.435(11)
Ba(1B)-O(7)#3	2.701(9)	B(3)-O(2)#10	1.448(12)
Ba(1B)-O(7)	2.848(9)	B(3)-O(5)	1.466(11)
Pb(2B)-O(10)	2.323(12)	B(3)-O(3)	1.508(11)
Pb(2B)-O(14)	2.437(17)	B(4)-O(8)	1.345(12)
Pb(2B)-O(5)	2.605(6)	B(4)-O(3)#11	1.374(12)
Ba(2)-O(6)#7	2.664(7)	B(4)-O(4B)	1.397(13)
Ba(2)-O(1)#7	2.728(6)	B(4)-O(4A)	1.397(13)
Ba(2)-O(5)	2.810(6)	B(5)-O(4A)#9	1.570(19)
Ba(2)-O(3)#8	2.843(6)	B(5)-O(7)	1.433(11)
Ba(2)-O(8)#8	2.893(7)	B(5)-O(9)	1.443(12)
Ba(2)-O(13)	2.946(9)	B(5)-O(4B)#9	1.365(18)
Ba(2)-O(2)#9	3.010(7)	Pb(1B)-O(9)	2.524(6)
Ba(2)-O(4B)#8	3.090(15)	B(6)#1-O(10)	1.354(8)
Ba(2)-O(3)	3.123(7)	O(13)-B(7)	1.374(8)
B(1)-O(5)	1.446(12)	O(12)-B(7)	1.374(8)
B(1)-O(1)	1.464(12)	O(12)-B(6)	1.354(8)
B(1)-O(6)	1.476(13)	B(7)-O(11)	1.374(8)
B(1)-O(8)	1.482(12)	O(14)-B(6)	1.354(8)
B(2)-O(6)#7	1.346(13)		
O(10)#1-Ba(1B)-O(9)	102.5(2)	O(3)#8-Ba(2)-O(3)	117.53(11)
O(10)#1-Ba(1B)-O(9)#2	102.6(2)	O(8)#8-Ba(2)-O(3)	101.15(17)
O(9)-Ba(1B)-O(9)#2	73.5(3)	O(13)-Ba(2)-O(3)	68.3(2)
O(10)#1-Ba(1B)-O(7)#3	112.1(3)	O(2)#9-Ba(2)-O(3)	71.35(16)
O(9)-Ba(1B)-O(7)#3	129.25(18)	O(4B)#8-Ba(2)-O(3)	100.8(3)
O(9)#2-Ba(1B)-O(7)#3	129.25(18)	O(5)-B(1)-O(1)	112.6(7)
O(10)#1-Ba(1B)-O(7)	145.1(3)	O(5)-B(1)-O(6)	112.6(8)
O(9)-Ba(1B)-O(7)	51.76(17)	O(1)-B(1)-O(6)	103.0(7)
O(9)#2-Ba(1B)-O(7)	51.76(17)	O(5)-B(1)-O(8)	109.3(7)
O(7)#3-Ba(1B)-O(7)	102.74(6)	O(1)-B(1)-O(8)	111.9(7)
O(10)-Pb(2B)-O(14)	81.5(4)	O(6)-B(1)-O(8)	107.3(8)
O(10)-Pb(2B)-O(5)	110.46(14)	O(6)#7-B(2)-O(1)	120.6(8)
O(14)-Pb(2B)-O(5)	115.2(4)	O(6)#7-B(2)-O(2)	120.0(9)
O(6)#7-Ba(2)-O(1)#7	50.5(2)	O(1)-B(2)-O(2)	119.3(8)
O(6)#7-Ba(2)-O(5)	66.2(2)	O(9)-B(3)-O(2)#10	109.7(8)
O(1)#7-Ba(2)-O(5)	113.74(18)	O(9)-B(3)-O(5)	109.7(7)
O(6)#7-Ba(2)-O(3)#8	72.5(2)	O(2)#10-B(3)-O(5)	111.3(7)

O(1)#7-Ba(2)-O(3)#8	60.53(17)	O(9)-B(3)-O(3)	109.9(7)
O(5)-Ba(2)-O(3)#8	119.69(18)	O(2)#10-B(3)-O(3)	107.2(7)
O(6)#7-Ba(2)-O(8)#8	139.5(2)	O(5)-B(3)-O(3)	108.9(7)
O(1)#7-Ba(2)-O(8)#8	96.79(19)	O(8)-B(4)-O(3)#11	123.3(9)
O(5)-Ba(2)-O(8)#8	148.96(18)	O(8)-B(4)-O(4B)	112.5(10)
O(3)#8-Ba(2)-O(8)#8	69.93(17)	O(3)#11-B(4)-O(4B)	122.8(10)
O(6)#7-Ba(2)-O(13)	110.8(3)	O(8)-B(4)-O(4A)	120.6(11)
O(1)#7-Ba(2)-O(13)	115.8(3)	O(3)#11-B(4)-O(4A)	115.0(10)
O(5)-Ba(2)-O(13)	67.6(3)	O(4A)#9-B(5)-O(7)	115.2(9)
O(3)#8-Ba(2)-O(13)	172.5(3)	O(4A)#9-B(5)-O(9)	115.8(9)
O(8)#8-Ba(2)-O(13)	104.9(3)	O(7)-B(5)-O(9)	110.4(8)
O(6)#7-Ba(2)-O(2)#9	98.5(2)	O(4A)#9-B(5)-O(4B)#9	21.5(7)
O(1)#7-Ba(2)-O(2)#9	108.13(17)	O(7)-B(5)-O(4B)#9	103.5(8)
O(5)-Ba(2)-O(2)#9	97.34(18)	O(9)-B(5)-O(4B)#9	107.2(9)
O(3)#8-Ba(2)-O(2)#9	47.89(18)	O(13)-B(7)-O(11)	120.01(10)
O(8)#8-Ba(2)-O(2)#9	66.39(19)	O(13)-B(7)-O(12)	120.01(10)
O(13)-Ba(2)-O(2)#9	136.0(3)	O(11)-B(7)-O(12)	119.98(10)
O(6)#7-Ba(2)-O(4B)#8	144.9(3)	O(10)#14-B(6)-O(14)	122.5(11)
O(1)#7-Ba(2)-O(4B)#8	98.5(3)	O(10)#14-B(6)-O(12)	114.6(10)
O(5)-Ba(2)-O(4B)#8	129.9(3)	O(14)-B(6)-O(12)	100.5(9)
O(3)#8-Ba(2)-O(4B)#8	109.2(3)	O(10)#1-Pb(1B)-O(9)	102.5(2)
O(8)#8-Ba(2)-O(4B)#8	44.6(2)	O(10)#1-Pb(1B)-O(9)#2	102.6(2)
O(13)-Ba(2)-O(4B)#8	64.1(3)	O(9)-Pb(1B)-O(9)#2	73.5(3)
O(2)#9-Ba(2)-O(4B)#8	108.2(2)	O(10)#1-Pb(1B)-O(7)#3	112.1(3)
O(6)#7-Ba(2)-O(3)	109.3(2)	O(9)-Pb(1B)-O(7)#3	129.25(18)
O(1)#7-Ba(2)-O(3)	159.78(16)	O(9)#2-Pb(1B)-O(7)#3	129.25(18)
O(5)-Ba(2)-O(3)	47.81(17)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,z-1/2 #2 -x+2,y,z #3 -x+2,-y,z-1/2

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

#8 -x+3/2,-y+1/2,z+1/2 #9 -x+3/2,y-1/2,z #10 x,-y+1,z-1/2

#11 -x+3/2,y+1/2,z #12 -x+3/2,-y+1/2,z-1/2 #13 -x+2,-y,z+1/2

#14 -x+2,-y+1,z+1/2 #15 x,y,z+1

Figure S1. Ball and stick structure of $Ba_2B_6O_{11}$. (a) $[B_3O_7]^{5-}$ group; (b) $[B_3O_8]^{7-}$ group; (c) the FBB $[B_6O_{14}]^{10-}$ formed by $[B_3O_7]^{5-}$ and $[B_3O_8]^{7-}$ group; (d) the two-dimensional layer $_\infty^2[B_6O_{10}]$; (e) the Ba1 and Ba2 cations filled the tunnels and interstices formed by $_\infty^2[B_6O_{10}]$ layers.