Supporting Information

$Pb_4Zn_2B_{10}O_{21}$: a congruently melting lead zinc borate with a novel $[B_{10}O_{24}]$ anionic group and an interesting $[Pb_4O_{12}]_\infty$ chain

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Pb_4Zn_2B_{10}O_{21}$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}	BVS
Pb(1)	-749(1)	9384(1)	4180(1)	13(1)	1.99
Pb(2)	-778(1)	6904(1)	4226(1)	14(1)	1.94
Pb(3)	701(1)	8324(1)	6185(1)	14(1)	1.92
Pb(4)	697(1)	5839(1)	5999(1)	15(1)	1.96
Zn(1)	2498(1)	4486(1)	7507(1)	7(1)	2.14
Zn(2)	2518(1)	6993(1)	7510(1)	7(1)	2.25
B(1)	763(9)	5459(6)	3632(9)	13(3)	3.01
B(2)	1666(7)	5789(6)	8618(8)	7(2)	3.12
B(3)	-641(8)	9489(6)	6718(9)	9(2)	3.01
B(4)	1627(7)	6734(6)	3568(8)	8(2)	3.01
B(5)	3387(7)	6757(6)	3553(8)	8(2)	3.08
B(6)	-623(8)	6998(6)	6739(8)	9(2)	2.98
B(7)	2533(7)	6820(6)	5177(9)	12(3)	3.07
B(8)	769(8)	7984(6)	3596(8)	11(2)	3.16
B(9)	3422(7)	5712(6)	8529(8)	4(2)	3.07
B(10)	2618(8)	4281(6)	5169(8)	10(2)	3.07
O(1)	2523(4)	8020(3)	8099(5)	7(2)	1.99
O(2)	2499(4)	5507(3)	8102(5)	7(2)	1.95
O(3)	-129(4)	9410(3)	5765(5)	9(1)	2.31
O(4)	-157(4)	6882(3)	5754(5)	10(1)	2.31
O(5)	1413(4)	4051(3)	8197(5)	10(1)	2.11
O(6)	3413(5)	5625(4)	9610(5)	14(2)	1.97
O(7)	1480(4)	6558(4)	8223(5)	11(1)	2.09
O(8)	3554(4)	6537(4)	8251(5)	11(1)	2.17
O(9)	-850(4)	7803(3)	6883(5)	9(1)	1.99
O(10)	3345(4)	6885(4)	4651(5)	12(2)	1.93
O(11)	0	6700(5)	7500	12(2)	2.04
O(12)	119(5)	5708(4)	4254(5)	16(2)	1.98
O(13)	0	9161(5)	7500	10(2)	2.07
O(14)	1805(4)	4189(4)	4722(5)	12(2)	1.99
O(15)	852(4)	7218(3)	3330(5)	11(1)	1.98
O(16)	-863(4)	5308(4)	6603(5)	10(1)	2.04
O(17)	60(5)	8201(4)	4150(5)	14(2)	2.02
O(18)	3511(4)	4046(3)	8286(5)	8(1)	2.11
O(19)	-850(4)	10289(3)	6925(5)	10(1)	1.87
O(20)	1724(5)	6694(4)	4675(5)	18(2)	1.91
O(21)	2740(6)	4258(4)	6172(6)	25(2)	1.93
O(22)	2518(6)	6889(6)	6154(8)	44(3)	2.06

Table S2. Selected bond distances (Å) and angles (deg) for $Pb_4Zn_2B_{10}O_{21}$.

Pb(1)-O(3)	2.294(7)	O(13)-Pb(3)-O(9)#2	64.56(18)
Pb(1)-O(17)	2.382(6)	O(9)-Pb(3)-O(9)#2	67.6(2)
Pb(1)-O(3)#1	2.470(6)	O(4)-Pb(4)-O(12)	75.5(2)
Pb(2)-O(4)	2.225(7)	O(4)-Pb(4)-O(16)	81.2(2)
Pb(2)-O(12)	2.469(7)	O(12)-Pb(4)-O(16)	87.6(2)
Pb(2)-O(17)	2.579(6)	O(4)-Pb(4)-O(11)	56.1(2)
Pb(2)-O(15)	2.718(6)	O(12)-Pb(4)-O(11)	127.97(17)
Pb(3)-O(3)	2.321(6)	O(16)-Pb(4)-O(11)	68.82(18)
Pb(3)-O(13)	2.499(5)	O(4)-Pb(4)-O(20)	76.6(2)
Pb(3)-O(9)	2.612(6)	O(12)-Pb(4)-O(20)	68.7(2)
Pb(3)-O(9)#2	2.735(6)	O(16)-Pb(4)-O(20)	150.8(2)
Pb(4)-O(4)	2.234(6)	O(11)-Pb(4)-O(20)	112.1(2)
Pb(4)-O(12)	2.479(7)	O(21)-Zn(1)-O(2)	125.8(3)
Pb(4)-O(16)	2.587(7)	O(21)-Zn(1)-O(18)	106.1(3)
Pb(4)-O(11)	2.699(5)	O(2)-Zn(1)-O(18)	98.3(3)
Pb(4)-O(20)	2.754(7)	O(21)-Zn(1)-O(5)	120.8(3)
Zn(1)-O(21)	1.854(8)	O(2)-Zn(1)-O(5)	99.4(3)
Zn(1)-O(2)	1.953(6)	O(18)-Zn(1)-O(5)	102.0(3)
Zn(1)-O(18)	1.963(6)	O(22)-Zn(2)-O(7)	116.5(3)
Zn(1)-O(5)	1.983(6)	O(22)-Zn(2)-O(1)	119.3(4)
Zn(2)-O(22)	1.812(10)	O(7)-Zn(2)-O(1)	99.6(3)
Zn(2)-O(7)	1.943(6)	O(22)-Zn(2)-O(8)	117.2(3)
Zn(2)-O(1)	1.959(6)	O(7)-Zn(2)-O(8)	101.3(3)
Zn(2)-O(8)	1.975(6)	O(1)-Zn(2)-O(8)	99.7(3)
B(1)-O(12)	1.326(14)	O(12)-B(1)-O(16)#3	122.2(10)
B(1)-O(16)#3	1.386(13)	O(12)-B(1)-O(5)#4	122.5(9)
B(1)-O(5)#4	1.404(13)	O(16)#3-B(1)-O(5)#4	115.3(9)
B(2)-O(7)	1.469(12)	O(7)-B(2)-O(16)#2	107.7(8)
B(2)-O(16)#2	1.473(12)	O(7)-B(2)-O(2)	107.0(8)
B(2)-O(2)	1.481(12)	O(16)#2-B(2)-O(2)	111.8(8)
B(2)-O(14)#5	1.483(12)	O(7)-B(2)-O(14)#5	110.8(8)
B(3)-O(19)	1.458(12)	O(16)#2-B(2)-O(14)#5	108.7(8)
B(3)-O(18)#6	1.462(12)	O(2)-B(2)-O(14)#5	110.7(8)
B(3)-O(3)	1.478(13)	O(19)-B(3)-O(18)#6	109.4(8)
B(3)-O(13)	1.511(12)	O(19)-B(3)-O(3)	110.9(8)
B(4)-O(15)	1.448(12)	O(18)#6-B(3)-O(3)	112.1(8)
B(4)-O(1)#7	1.456(12)	O(19)-B(3)-O(13)	111.4(8)
B(4)-O(20)	1.481(13)	O(18)#6-B(3)-O(13)	109.1(7)
B(4)-O(5)#4	1.491(12)	O(3)-B(3)-O(13)	104.0(7)
B(5)-O(18)#4	1.460(12)	O(15)-B(4)-O(1)#7	113.6(8)
B(5)-O(9)#8	1.473(12)	O(15)-B(4)-O(20)	108.6(8)
B(5)-O(10)	1.477(13)	O(1)#7-B(4)-O(20)	111.0(8)
B(5)-O(1)#7	1.511(12)	O(15)-B(4)-O(5)#4	107.7(8)

B(6)-O(11)	1.457(11)	O(1)#7-B(4)-O(5)#4	108.0(8)
B(6)-O(9)	1.459(12)	O(20)-B(4)-O(5)#4	107.8(8)
B(6)-O(7)#2	1.470(12)	O(18)#4-B(5)-O(9)#8	108.3(8)
B(6)-O(4)	1.489(13)	O(18)#4-B(5)-O(10)	113.0(8)
B(7)-O(22)	1.305(15)	O(9)#8-B(5)-O(10)	110.0(8)
B(7)-O(20)	1.375(13)	O(18)#4-B(5)-O(1)#7	105.0(7)
B(7)-O(10)	1.382(12)	O(9)#8-B(5)-O(1)#7	111.9(7)
B(8)-O(17)	1.327(13)	O(10)-B(5)-O(1)#7	108.6(8)
B(8)-O(8)#7	1.374(13)	O(11)-B(6)-O(9)	113.3(8)
B(8)-O(15)	1.391(13)	O(11)-B(6)-O(7)#2	108.7(8)
B(9)-O(19)#9	1.430(12)	O(9)-B(6)-O(7)#2	107.8(8)
B(9)-O(6)	1.445(12)	O(11)-B(6)-O(4)	106.1(7)
B(9)-O(8)	1.502(12)	O(9)-B(6)-O(4)	110.5(8)
B(9)-O(2)	1.506(12)	O(7)#2-B(6)-O(4)	110.4(8)
B(10)-O(14)	1.337(13)	O(22)-B(7)-O(20)	118.9(9)
B(10)-O(21)	1.345(14)	O(22)-B(7)-O(10)	120.8(9)
B(10)-O(6)#4	1.389(13)	O(20)-B(7)-O(10)	120.3(9)
O(3)-Pb(1)-O(17)	80.6(2)	O(17)-B(8)-O(8)#7	124.9(9)
O(3)-Pb(1)-O(3)#1	75.6(2)	O(17)-B(8)-O(15)	119.0(9)
O(17)-Pb(1)-O(3)#1	119.0(2)	O(8)#7-B(8)-O(15)	116.1(9)
O(4)-Pb(2)-O(12)	75.8(2)	O(19)#9-B(9)-O(6)	111.9(8)
O(4)-Pb(2)-O(17)	81.8(2)	O(19)#9-B(9)-O(8)	107.3(7)
O(12)-Pb(2)-O(17)	119.6(2)	O(6)-B(9)-O(8)	110.3(7)
O(4)-Pb(2)-O(15)	92.7(2)	O(19)#9-B(9)-O(2)	112.6(7)
O(12)-Pb(2)-O(15)	73.3(2)	O(6)-B(9)-O(2)	110.0(8)
O(17)-Pb(2)-O(15)	52.4(2)	O(8)-B(9)-O(2)	104.5(7)
O(3)-Pb(3)-O(13)	58.4(2)	O(14)-B(10)-O(21)	123.7(10)
O(3)-Pb(3)-O(9)	85.3(2)	O(14)-B(10)-O(6)#4	121.2(9)
O(13)-Pb(3)-O(9)	66.45(19)	O(21)-B(10)-O(6)#4	115.0(9)
O(3)-Pb(3)-O(9)#2	122.7(2)		

Note. Symmetry transformations used to generate equivalent atoms:

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

#5 x-1/2,-y+1/2,-z+1 #6 -x+3/2,-y+1/2,z-1/2 #7 x,-y+1,z+1/2 #8 -x+3/2,y+1/2,z

#9 -x+3/2,y-1/2,z #10 -x+2,y,-z+3/2 #11 x,-y+1,z-1/2

Figure S1. The infrared spectrum of $Pb_4Zn_2B_{10}O_{21}$.