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$Pb_{10}O_4(BO_3)_3I_3$: A New Noncentrosymmetric Oxyborate Iodide Synthesized by the Straightforward Hydrothermal Method

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Table S1. Crystal Data and Structure Refinement for $Pb_{10}O_4(BO_3)_3I_3$.

Empirical formula	$Pb_{10}O_4(BO_3)_3I_3$
Formula weight	2693.03
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*Cc*
Unit cell dimensions	a = 16.6423(5) Å b = 9.0277(3) Å c = 16.9746(5) Å β = 115.6580(10)°
Volume	2298.82(12) $Å^3$
Z	4
Density (g/cm^3)	7.781
Absorption coefficient (mm^{-1})	77.019
F(000)	4392
Theta range for data collection	2.63 to 27.50
Limiting indices	$-21 \le h \le 21$, $-10 \le k \le 11$, $-22 \le l \le 22$
Reflections collected / unique	16455/5081[R_{int} = 0.0455]
Completeness to theta	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5081 / 80 / 264
Goodness-of-fit on F^2	1.043
Final R indices [$F_o^2 > 2\sigma(F_o^2)$][a]	R_1 = 0.0247 wR_2 = 0.0553
R indices (all data)[a]	R_1 =0.0261 wR_2 = 0.0559
Absolute structure parameter	0.368(8)
Extinction coefficient	0.000035(5)
Largest diff. peak and hole	2.829 and -1.696 e·$Å^{-3}$

Table S2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2$ × 10^3) for $Pb_{10}O_4(BO_3)_3I_3$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x	y	z	U(eq)	BVS
Pb(1)	6714(1)	4692(1)	2192(1)	8(1)	1.985
Pb(2)	7842(1)	10395(1)	3170(1)	6(1)	2.197
Pb(3)	11150(1)	15320(1)	4279(1)	7(1)	1.955
Pb(4)	10024(1)	9681(1)	3276(1)	6(1)	1.985
Pb(5)	9894(1)	12534(1)	4896(1)	7(1)	1.827
Pb(6)	8029(1)	7474(1)	1605(1)	6(1)	1.825
Pb(7)	9158(1)	13516(1)	2666(1)	7(1)	1.955
Pb(8)	8765(1)	6633(1)	3913(1)	6(1)	1.952
Pb(9)	5587(1)	8216(1)	1222(1)	8(1)	2.124
Pb(10)	12403(1)	11609(1)	5340(1)	9(1)	2.165
I(1)	7713(1)	6495(1)	9323(1)	10(1)	0.7807
I(2)	200(1)	3527(1)	7146(1)	10(1)	0.7437
I(3)	8982(1)	9568(1)	5794(1)	11(1)	0.5109
B(1)	6449(13)	7500(20)	3330(11)	5(2)	3.031
B(2)	6982(12)	10900(20)	1311(11)	7(3)	2.908
B(3)	5919(14)	5870(20)	82(14)	19(4)	3.010
O(1)	9185(7)	11492(12)	3568(7)	6(2)	2.394
O(2)	8675(8)	8560(13)	2920(8)	10(2)	2.3834
O(3)	10386(7)	8167(13)	4489(7)	7(2)	1.997
O(4)	7480(9)	11815(15)	1971(9)	17(3)	2.014
O(5)	11002(7)	10588(13)	4866(7)	10(2)	2.105
O(6)	11571(7)	13585(12)	5434(7)	4(2)	2.170
O(7)	8069(7)	5531(12)	2576(7)	7(2)	2.237
O(8)	9768(6)	14646(11)	4039(7)	7(2)	2.244
O(9)	6363(8)	6301(13)	950(8)	12(2)	2.161
O(10)	6895(8)	9423(13)	1471(8)	10(2)	2.075
O(11)	6374(6)	7081(11)	2505(7)	12(2)	2.144
O(12)	5794(7)	8238(12)	3406(8)	17(2)	2.088
O(13)	7252(6)	7259(11)	4034(6)	11(2)	2.007

Table S3. Selected bond distances (Å) and angles (deg) for $Pb_{10}O_4(BO_3)_3I_3$.

Pb(1)-O(7)	2.193(10)	O(7)-Pb(6)-O(9)	73.4(3)
Pb(1)-O(11)	2.349(10)	O(10)-Pb(6)-O(9)	69.1(4)
Pb(1)-O(9)	2.414(12)	O(8)-Pb(7)-O(1)	79.3(4)
Pb(2)-O(4)	2.255(14)	O(8)-Pb(7)-O(12)#1	68.3(4)
Pb(2)-O(1)	2.264(11)	O(1)-Pb(7)-O(12)#1	83.4(4)
Pb(2)-O(2)	2.316(12)	O(8)-Pb(7)-O(7)#4	74.7(3)
Pb(3)-O(8)	2.240(10)	O(1)-Pb(7)-O(7)#4	114.0(4)
Pb(3)-O(12)#1	2.307(11)	O(12)#1-Pb(7)-O(7)#4	135.2(3)
Pb(3)-O(6)	2.366(11)	O(7)-Pb(8)-O(2)	76.4(4)
Pb(3)-I(2)#2	3.4248(12)	O(7)-Pb(8)-O(8)#5	78.2(3)
Pb(4)-O(2)	2.292(12)	O(2)-Pb(8)-O(8)#5	115.9(4)
Pb(4)-O(3)	2.324(11)	O(7)-Pb(8)-O(13)	94.6(3)
Pb(4)-O(1)	2.339(11)	O(2)-Pb(8)-O(13)	97.4(4)
Pb(4)-O(5)	2.608(11)	O(8)#5-Pb(8)-O(13)	142.6(3)
Pb(5)-O(1)	2.249(11)	O(11)-Pb(9)-O(10)	86.0(4)
Pb(5)-O(8)	2.352(10)	O(11)-Pb(9)-O(9)	73.2(4)
Pb(5)-O(5)	2.563(11)	O(10)-Pb(9)-O(9)	80.0(4)
Pb(5)-O(6)	2.705(11)	O(13)#1-Pb(10)-O(5)	95.6(4)
Pb(6)-O(2)	2.240(12)	O(13)#1-Pb(10)-O(6)	93.1(4)
Pb(6)-O(7)	2.387(10)	O(5)-Pb(10)-O(6)	77.7(4)
Pb(6)-O(10)	2.516(12)	O(12)-B(1)-O(13)	121.7(15)
Pb(6)-O(9)	2.716(13)	O(12)-B(1)-O(11)	120.6(15)
Pb(7)-O(8)	2.335(10)	O(13)-B(1)-O(11)	117.3(15)
Pb(7)-O(1)	2.371(11)	O(4)-B(2)-O(10)	120.3(15)
Pb(7)-O(12)#1	2.469(10)	O(4)-B(2)-O(6)#7	121.2(15)
Pb(7)-O(7)#4	2.525(10)	O(10)-B(2)-O(6)#7	118.4(14)
Pb(8)-O(7)	2.282(10)	O(3)#8-B(3)-O(9)	119.3(17)
Pb(8)-O(2)	2.381(12)	O(3)#8-B(3)-O(5)#8	121.9(17)
Pb(8)-O(8)#5	2.397(10)	O(9)-B(3)-O(5)#8	118.7(17)
Pb(8)-O(13)	2.674(10)	O(3)#8-B(3)-Pb(4)#8	55.2(9)
Pb(9)-O(11)	2.245(10)	O(9)-B(3)-Pb(4)#8	173.7(15)
Pb(9)-O(10)	2.305(12)	O(5)#8-B(3)-Pb(4)#8	67.1(9)
Pb(9)-O(9)	2.321(11)	Pb(5)-O(1)-Pb(2)	120.2(5)
Pb(10)-O(13)#1	2.200(10)	Pb(5)-O(1)-Pb(4)	113.7(5)
Pb(10)-O(5)	2.304(12)	Pb(2)-O(1)-Pb(4)	103.5(4)
Pb(10)-O(6)	2.306(11)	Pb(5)-O(1)-Pb(7)	100.4(4)
I(2)-Pb(3)#6	3.4248(12)	Pb(2)-O(1)-Pb(7)	113.9(5)
B(1)-O(12)	1.33(2)	Pb(4)-O(1)-Pb(7)	104.4(5)
B(1)-O(13)	1.37(2)	Pb(6)-O(2)-Pb(4)	116.7(6)
B(1)-O(11)	1.40(2)	Pb(6)-O(2)-Pb(2)	115.3(5)
B(2)-O(4)	1.35(2)	Pb(4)-O(2)-Pb(2)	103.4(5)
B(2)-O(10)	1.38(2)	Pb(6)-O(2)-Pb(8)	104.0(5)
B(2)-O(6)#7	1.42(2)	Pb(4)-O(2)-Pb(8)	112.5(5)

B(3)-O(3)#8	1.34(2)	Pb(2)-O(2)-Pb(8)	104.6(5)
B(3)-O(9)	1.39(2)	B(3)#3-O(3)-Pb(4)	96.7(11)
B(3)-O(5)#8	1.39(2)	B(2)-O(4)-Pb(2)	103.4(11)
O(3)-B(3)#3	1.34(2)	B(3)#3-O(5)-Pb(10)	119.2(11)
O(5)-B(3)#3	1.39(2)	B(3)#3-O(5)-Pb(5)	119.3(12)
O(6)-B(2)#9	1.42(2)	Pb(10)-O(5)-Pb(5)	110.3(4)
O(7)-Pb(7)#5	2.525(10)	B(3)#3-O(5)-Pb(4)	83.6(10)
O(8)-Pb(8)#4	2.397(10)	Pb(10)-O(5)-Pb(4)	124.8(5)
O(12)-Pb(3)#10	2.307(11)	Pb(5)-O(5)-Pb(4)	96.0(3)
O(12)-Pb(7)#10	2.469(10)	B(2)#9-O(6)-Pb(10)	107.0(9)
O(13)-Pb(10)#10	2.200(10)	B(2)#9-O(6)-Pb(3)	119.3(9)
O(7)-Pb(1)-O(11)	86.2(4)	Pb(10)-O(6)-Pb(3)	115.2(5)
O(7)-Pb(1)-O(9)	83.2(4)	B(2)#9-O(6)-Pb(5)	115.2(10)
O(11)-Pb(1)-O(9)	69.8(4)	Pb(10)-O(6)-Pb(5)	105.5(4)
O(4)-Pb(2)-O(1)	82.2(4)	Pb(3)-O(6)-Pb(5)	93.5(3)
O(4)-Pb(2)-O(2)	100.8(5)	Pb(1)-O(7)-Pb(8)	117.4(5)
O(1)-Pb(2)-O(2)	77.0(4)	Pb(1)-O(7)-Pb(6)	109.3(4)
O(8)-Pb(3)-O(12)#1	72.8(4)	Pb(8)-O(7)-Pb(6)	102.5(4)
O(8)-Pb(3)-O(6)	83.3(4)	Pb(1)-O(7)-Pb(7)#5	112.8(4)
O(12)#1-Pb(3)-O(6)	84.0(4)	Pb(8)-O(7)-Pb(7)#5	102.2(4)
O(8)-Pb(3)-I(2)#2	85.6(3)	Pb(6)-O(7)-Pb(7)#5	112.1(4)
O(12)#1-Pb(3)-I(2)#2	72.3(3)	Pb(3)-O(8)-Pb(7)	105.6(4)
O(6)-Pb(3)-I(2)#2	155.9(3)	Pb(3)-O(8)-Pb(5)	107.4(4)
O(2)-Pb(4)-O(3)	79.7(4)	Pb(7)-O(8)-Pb(5)	98.5(4)
O(2)-Pb(4)-O(1)	76.0(4)	Pb(3)-O(8)-Pb(8)#4	115.7(4)
O(3)-Pb(4)-O(1)	99.9(4)	Pb(7)-O(8)-Pb(8)#4	104.6(4)
O(2)-Pb(4)-O(5)	120.8(4)	Pb(5)-O(8)-Pb(8)#4	122.3(4)
O(3)-Pb(4)-O(5)	57.4(4)	B(3)-O(9)-Pb(9)	109.6(11)
O(1)-Pb(4)-O(5)	73.9(4)	B(3)-O(9)-Pb(1)	125.0(12)
O(2)-Pb(4)-B(3)#3	101.9(6)	Pb(9)-O(9)-Pb(1)	102.7(5)
O(3)-Pb(4)-B(3)#3	28.2(5)	B(3)-O(9)-Pb(6)	121.6(12)
O(1)-Pb(4)-B(3)#3	88.6(5)	Pb(9)-O(9)-Pb(6)	100.7(4)
O(5)-Pb(4)-B(3)#3	29.3(5)	Pb(1)-O(9)-Pb(6)	93.4(4)
O(1)-Pb(5)-O(8)	81.4(4)	B(2)-O(10)-Pb(9)	126.2(10)
O(1)-Pb(5)-O(5)	76.3(4)	B(2)-O(10)-Pb(6)	123.7(10)
O(8)-Pb(5)-O(5)	114.6(4)	Pb(9)-O(10)-Pb(6)	107.3(5)
O(1)-Pb(5)-O(6)	120.1(4)	B(1)-O(11)-Pb(9)	127.4(10)
O(8)-Pb(5)-O(6)	74.2(3)	B(1)-O(11)-Pb(1)	123.2(10)
O(5)-Pb(5)-O(6)	66.5(3)	Pb(9)-O(11)-Pb(1)	107.2(4)
O(2)-Pb(6)-O(7)	77.1(4)	B(1)-O(12)-Pb(3)#10	118.5(10)
O(2)-Pb(6)-O(10)	78.6(4)	B(1)-O(12)-Pb(7)#10	140.5(11)
O(7)-Pb(6)-O(10)	111.9(4)	Pb(3)#10-O(12)-Pb(7)#10	99.4(4)
O(2)-Pb(6)-O(9)	122.9(4)	B(1)-O(13)-Pb(10)#10	124.3(10)
		B(1)-O(13)-Pb(8)	124.2(10)

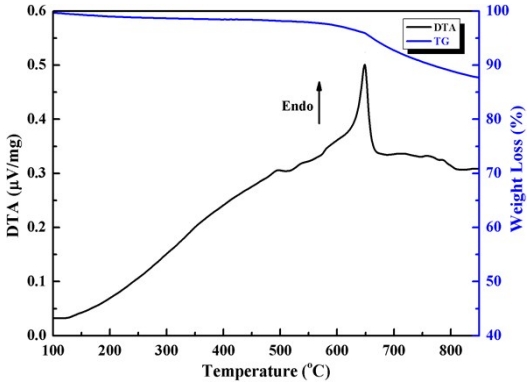
	Pb(10)#10-O(13)-Pb(8)	108.7(4)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,y+1/2,z #2 x+1,-y+2,z-1/2
#3 x+1/2,-y+3/2,z+1/2 #4 x,y+1,z
#5 x,y-1,z #6 x-1,-y+2,z+1/2 #7 x-1/2,-y+5/2,z-1/2
#8 x-1/2,-y+3/2,z-1/2 #9 x+1/2,-y+5/2,z+1/2
#10 x-1/2,y-1/2,z

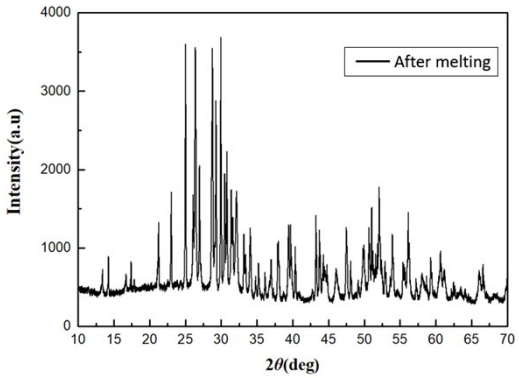
Table S4. The dipole moments of BO_3.

Repeating units	Polyhedron	X-axis Dipole moment	Y-axis Dipole moment	Z-axis Dipole moment
BO_3	$B(1)O_3$	1.103519	-0.96203	-0.58298
	$B(2)O_3$	0.268616	-0.39973	-0.55312
	$B(3)O_3$	-0.35877	0.366225	0.799839

Figure S1. The thermal analysis of $Pb_{10}O_4(BO_3)_3I_3$: (a) The TG-DSC curves of polycrystalline sample of $Pb_{10}O_4(BO_3)_3I_3$. (b) The powder XRD patterns of the residual after TG/DTA for $Pb_{10}O_4(BO_3)_3I_3$.



(a)



(b)

Figure S2. The direction of the dipole moment of the repeating unit $[Pb_{10}O_8]$.

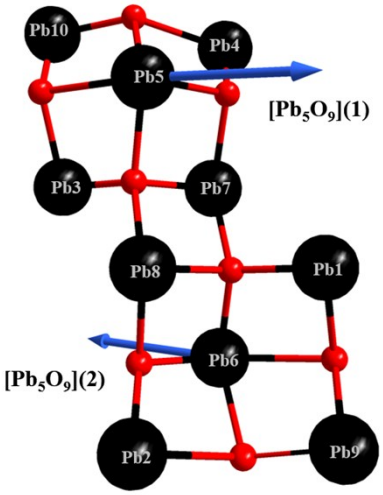


Figure S3. The dipole moments direction of BO_3 groups in the unit cell.