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Electronic Supplementary Information

$[O_2Pb_3]_2(BO_3)I$: A New Lead Borate Iodide with $^1_\infty[O2Pb3]$ Double Chains

Kuan Li,[a] Alimujiang Yalikun[b] and Zhi Su [a*]

[a]College of Chemistry and Chemical Engineering, Xinjiang Normal University, Urumqi, Xinjiang 830054, P. R. China.

[b]School of Physics and Technology, Xinjiang University, Urumqi, Xinjiang 830046, P. R. China.

*Corresponding author, e-mail: suzhixj@sina.com

Table S1 Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and bond valence sums (BVS) calculations for $[O_2Pb_3]_2(BO_3)I$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	*x*	*y*	*z*	$U_{(eq)}$	BVS
Pb(1)	7500	5206(1)	3823(1)	20(1)	1.7
Pb(2)	2500	4549(1)	1651(2)	19(1)	2.1
Pb(3)	7500	7500	1287(2)	18(1)	2.1
Pb(4)	2500	7500	3582(2)	17(1)	1.9
B(1)	2500	2500	4070(70)	32(16)	2.9
O(1)	10(20)	6068(12)	2459(14)	13(3)	2.1
O(2)	2500	2500	5470(30)	25(8)	1.6
O(3)	2500	3770(20)	3580(20)	25(6)	1.7
I(1)	7500	2500	1166(4)	40(1)	0.8

Table S2 Selected bond lengths (Å) and angles (°) for $[O_2Pb_3]_2(BO_3)I$.

Pb(1)-O(1)#1	2.216(15)	Pb(3)-O(1)#5	2.365(14)
Pb(1)-O(1)#2	2.216(15)	Pb(3)-O(1)#2	2.365(14)
Pb(1)-O(2)#3	2.355(12)	Pb(3)-I(1)	3.893(3)
Pb(1)-I(1)	3.851(2)	Pb(4)-O(1)#5	2.331(14)
Pb(2)-O(3)	2.19(3)	Pb(4)-O(1)#7	2.331(14)
Pb(2)-O(1)#1	2.233(13)	Pb(4)-O(1)#1	2.331(14)
Pb(2)-O(1)	2.233(13)	Pb(4)-O(1)	2.331(14)
Pb(2)-I(1)	3.547(4)	B(1)-O(3)#9	1.33(3)
Pb(3)-O(1)#4	2.365(14)	B(1)-O(3)	1.33(3)
Pb(3)-O(1)#1	2.365(14)	B(1)-O(2)	1.48(7)
O(1)#1-Pb(1)-O(1)#2	81.8(7)	O(1)#5-Pb(3)-O(1)#2	116.5(7)
O(1)#1-Pb(1)-O(2)#3	81.5(7)	O(1)#5-Pb(4)-O(1)#7	76.2(7)
O(1)#2-Pb(1)-O(2)#3	81.5(7)	O(1)#5-Pb(4)-O(1)#1	73.4(6)
O(3)-Pb(2)-O(1)#1	82.5(6)	O(1)#7-Pb(4)-O(1)#1	118.4(7)
O(3)-Pb(2)-O(1)	82.5(6)	O(1)#5-Pb(4)-O(1)	118.4(7)
O(1)#1-Pb(2)-O(1)	80.2(7)	O(1)#7-Pb(4)-O(1)	73.4(6)
O(1)#4-Pb(3)-O(1)#1	116.5(7)	O(1)#1-Pb(4)-O(1)	76.2(7)
O(1)#4-Pb(3)-O(1)#5	75.7(7)	O(3)#9-B(1)-O(3)	134(6)
O(1)#1-Pb(3)-O(1)#5	72.1(6)	O(3)#9-B(1)-O(2)	113(3)
O(1)#4-Pb(3)-O(1)#2	72.1(6)	O(3)-B(1)-O(2)	113(3)
O(1)#1-Pb(3)-O(1)#2	75.7(7)		

Symmetry transformations used to generate equivalent atoms:

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

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

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

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

Table S3 The birefringence (Δn) and contribution percent w (%) of different units in $[O_2Pb_3]_2(BO_3)I$ calculated by the real space atom cutting method.

Units	Δn	w (%)
$[BO_3]$	0.027	27.8
I	0.034	35.1
Pb–O polyhedron	0.036	37.1

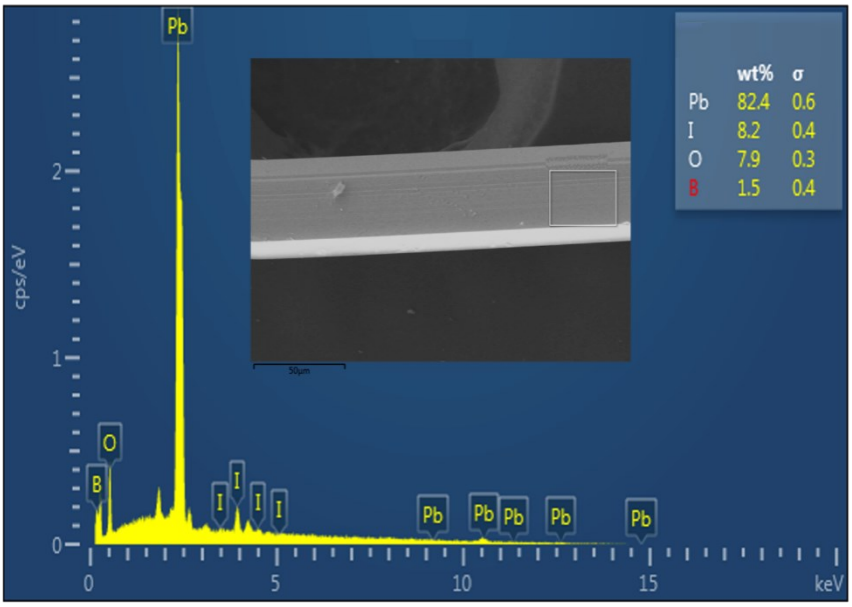

Figure S1 EDS of $[O_2Pb_3]_2(BO_3)I$ crystal which confirmed the existence of the Pb, B, O and I elements.

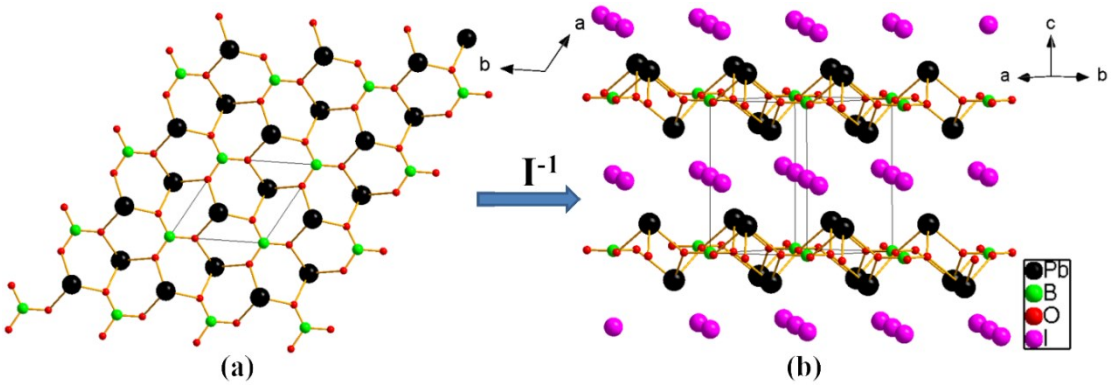

Figure S2 Crystal structure of Pb_2BO_3I. (a) 2D $^{2}_{\infty}[Pb2BO3]$ layer viewing along the c-axis; (b) Final structure of Pb_2BO_3I with the I^- ions located between the $^{2}_{\infty}[Pb2BO3]$ layers.

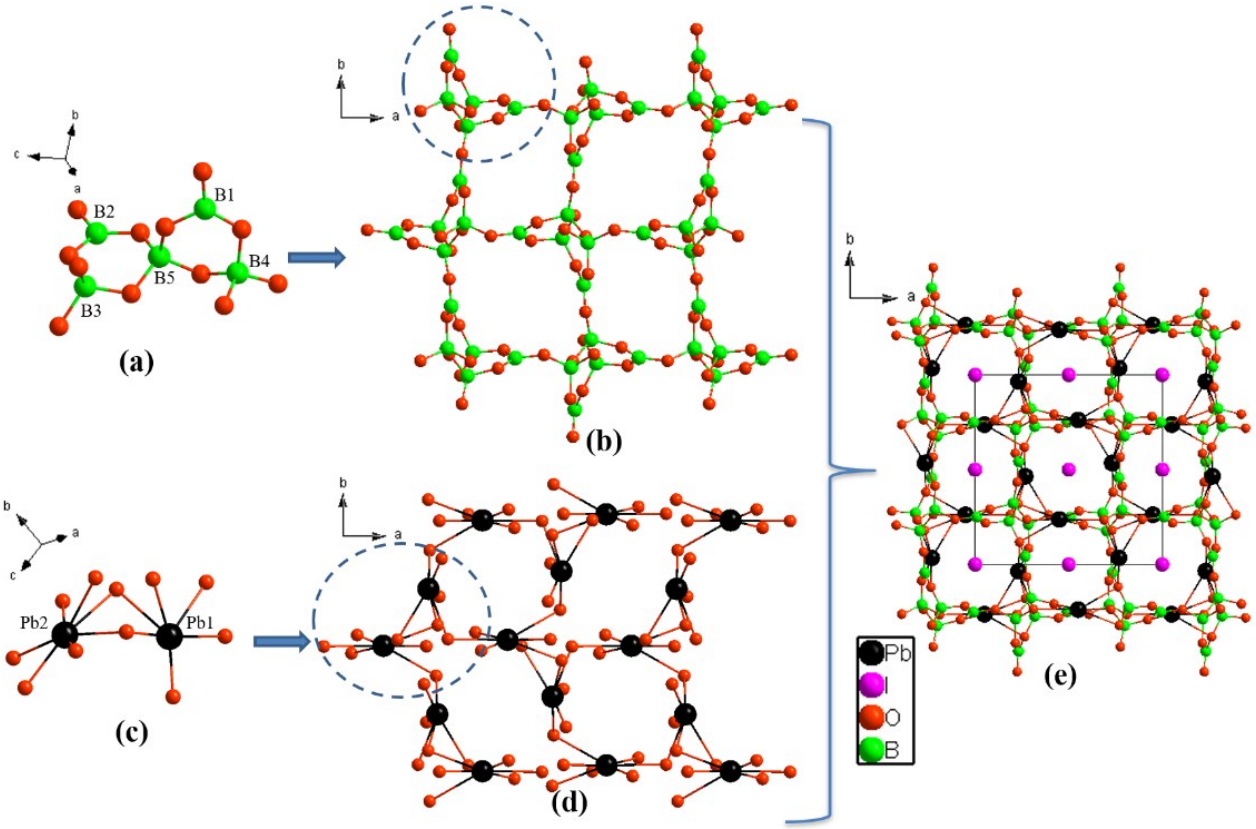

Figure S3 Crystal structure of $Pb_2B_5O_9I$. (a) $[B_5O_9]$ FBB; (b) 3D $^{3}_{\infty}[B5O9]$ anion framework; (c) Coordination environment of the Pb ions; (d) 3D framework composed by the Pb-O polyhedra; (c) Final structure of $Pb_2B_5O_9I$ with the I^- ions filled in the tunnels viewing along the c-axis .

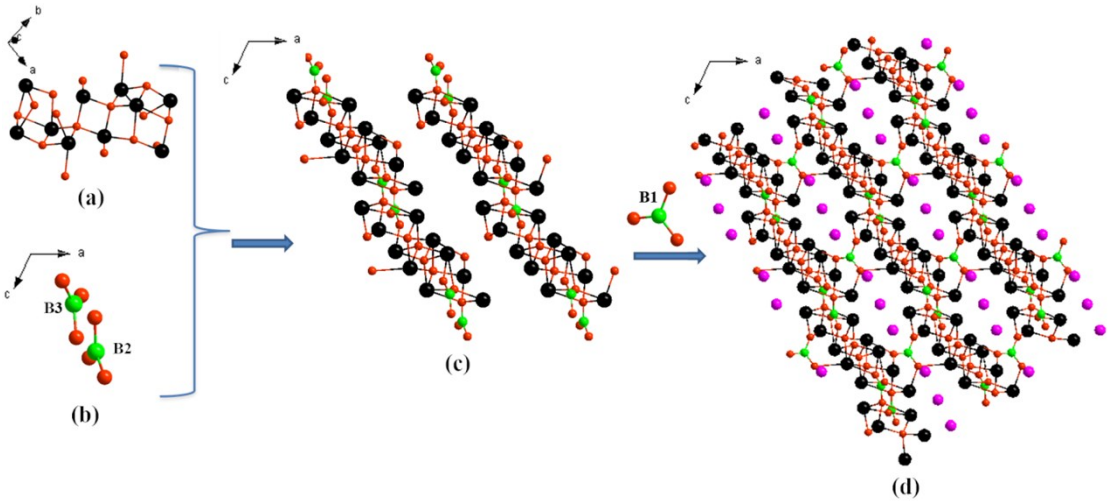

Figure S4 Crystal structure of $Pb_{10}O_4(BO_3)_3I_3$. (a) $[Pb_{10}O_8]$ repeating units; (b) BO_3 triangle; (c) 2D $^{2}_{\infty}$[Pb10O8(BO3)2] layers; (d) 3D $^{3}_{\infty}$[Pb10O4(BO3)3] framework with I^- ions filled in the interlayers.

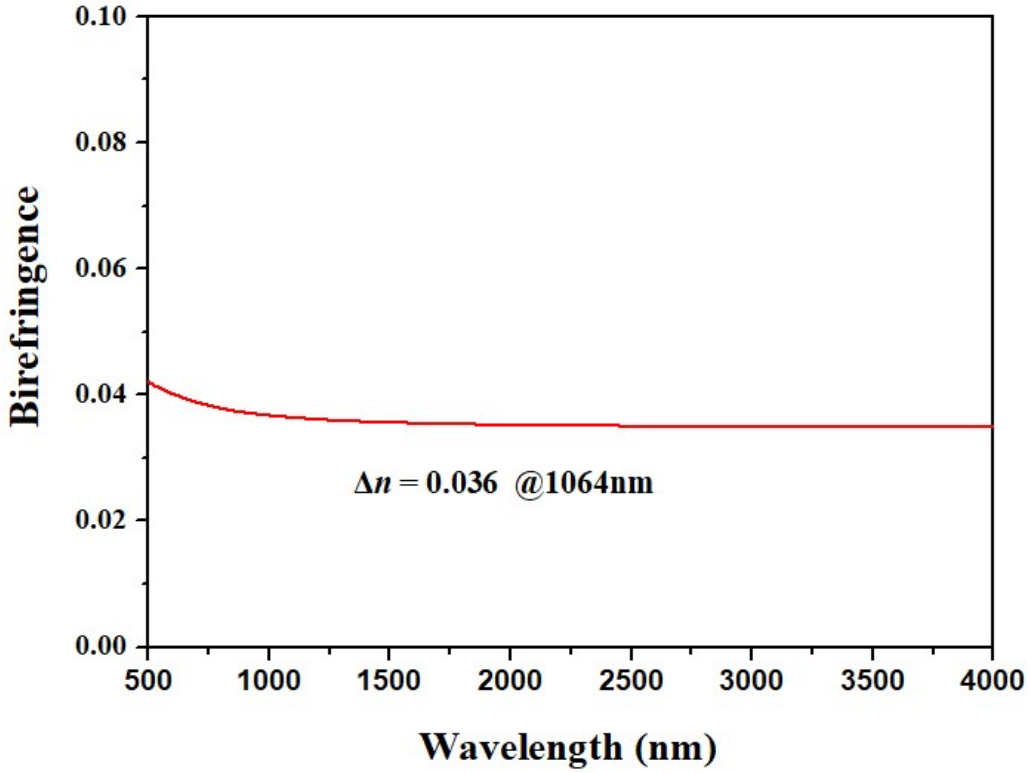

Figure S5 The birefringence (Δn) curve for $[O_2Pb_3]_2(BO_3)Br$.