## **Supporting Information for:**

## A Facile Strategy to Adjust the Density of Planar Triangle Units in Lead Borate-Nitrates

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**Table S1.** The amount of starting materials used in this study.

**Table S2.** Bond distances (Å) and angles [°] for  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$ .

**Table S3.** Bond distances (Å) and angles [°] for  $H[Pb_6(\mu_3-O)_2(BO_3)_2](NO_3)_3$ .

**Table S4.** Bond distances (Å) and angles [°] for H[Pb<sub>8</sub>( $\mu_4$ -O)<sub>3</sub>( $\mu_3$ -O)(BO<sub>3</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub>.

Chart S1. The products obtained at different reaction condition.

**Chart S2.** Molar ratio of  $Pb^{2+}/(BO_2)^{-1}$  under different pH Values.

Figure S1. Experimental and calculated powder X-ray diffraction patterns of  $[Pb_6(\mu_4-$ 

O)<sub>4</sub>(BO<sub>3</sub>)](NO<sub>3</sub>) (**a**), H[Pb<sub>6</sub>( $\mu_3$ -O)<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub> (**b**) and H[Pb<sub>8</sub>( $\mu_4$ -

$$O_{3}(\mu_{3}-O)(BO_{3})_{2}](NO_{3})_{3}(c), Pb_{2}(BO_{3})(NO_{3})(d) and Pb_{4}(NO_{3})_{4}(OH)_{4}(e).$$

Figure S2. UV-vis-NIR absorption spectra of  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$  (a),  $H[Pb_6(\mu_3-D)_4(BO_3)](NO_3)$  (b),  $H[Pb_6(\mu_3-D)_4(BO_3)](NO_3)$  (b),  $H[Pb_6(\mu_3-D)_4(BO_3)](NO_3)$  (c),  $H[Pb_6(\mu_3-D)_4(BO_3)$ 

 $O_{2}(BO_{3})_{2}(NO_{3})_{3}(\mathbf{b})$  and  $H[Pb_{8}(\mu_{4}-O_{3}(\mu_{3}-O)(BO_{3})_{2}](NO_{3})_{3}(\mathbf{c}).$ 

Figure S3. IR spectra of  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$  (a),  $H[Pb_6(\mu_3-O)_2(BO_3)_2](NO_3)_3$ 

(**b**) and H[Pb<sub>8</sub>(
$$\mu_4$$
-O)<sub>3</sub>( $\mu_3$ -O)(BO<sub>3</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub>(**c**).

Table S1. The amount of starting materials used in this study.

Compound	Starting materials		
$[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$ (1)	PbO (0.5632 g)+Mg(BO <sub>2</sub> ) <sub>2</sub> ·H <sub>2</sub> O (0.1841 g)		
	and $HNO_3$ (0.2 mL) +12 mL $H_2O$		
H[Pb <sub>6</sub> ( $\mu_3$ -O) <sub>2</sub> (BO <sub>3</sub> ) <sub>2</sub> ](NO <sub>3</sub> ) <sub>3</sub> (2)	$Pb(NO_3)_2$ (0.5281 g) + $Mg(BO_2)_2 \cdot H_2O$		
	(0.1502 g) +12 mL H <sub>2</sub> O (12.0 mL)		
H[Pb <sub>8</sub> ( $\mu_4$ -O) <sub>3</sub> ( $\mu_3$ -O)(BO <sub>3</sub> ) <sub>2</sub> ](NO <sub>3</sub> ) <sub>3</sub> (3)	$Pb(NO_3)_2$ (0.4984 g)+ $Mg(BO_2)_2 \cdot H_2O$		
	$(0.1763 \text{ g}) + 6.0 \text{ mL H}_2\text{O}$		
Pb <sub>2</sub> (BO <sub>3</sub> )(NO <sub>3</sub> )	$Pb(NO_3)_2$ (0.4975 g) + Mg(BO_2)_2•H_2O		
	$(0.1756 \text{ g}) + 12 \text{ mL H}_2\text{O}$		
Pb <sub>4</sub> (NO <sub>3</sub> ) <sub>4</sub> (OH) <sub>4</sub>	$Pb(NO_3)_2 (0.6776 \text{ g}) + Mg(BO_2)_2 \cdot H_2O$		
	$(0.1243 \text{ g}) + 12 \text{ mL H}_2\text{O}$		

**Table S2.** Bond Distances (Å) and angles [°] for  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$ 

Pb(1)-O(1)	2.24(2)	Pb(4)-O(2)#7	2.356(10)
Pb(1)-O(2)	2.245(10)	Pb(4)-O(2)#3	2.356(10)
Pb(1)-O(2)#1	2.245(10)	Pb(4)-O(2)#5	2.356(10)
Pb(2)-O(2)#3	2.235(10)	B(1)-O(3)#9	1.35(5)
Pb(2)-O(2)	2.235(10)	B(1)-O(1)#2	1.38(3)
Pb(2)-O(3)	2.381(9)	B (1)-O(1)	1.38(3)
Pb(2)-Pb(4)	3.5679(15)	N(1)-O(4)#10	1.19(3)
Pb(3)-O(2)#1	2.342(10)	N(1)-O(4)	1.19(3)
Pb(3)-O(2)#5	2.342(10)	N(1)-O(5)	1.30(5)
Pb(3)-O(2)#6	2.342(10)	O(3)-B(1)#9	1.35(5)
Pb(3)-O(2)	2.342(10)	O(3)-Pb(2)#7	2.381(9)
Pb(4)-O(2)	2.356(10)		
O(1)-Pb(1)-O(2)	81.5(5)	O(2)-Pb(4)-O(2)#3	74.2(5)
O(1)-Pb(1)-O(2)#1	81.5(5)	B(1)#9-O(3)-Pb(2)	109.6(6)
O(2)-Pb(1)-O(2)#1	80.8(5)	B(1)#9-O(3)-Pb(2)#7	109.6(6)
O(2)#3-Pb(2)-O(2)	79.0(5)	Pb(2)-O(3)-Pb(2)#7	140.9(13)
O(2)#3-Pb(2)-O(3)	81.6(6)	Pb(2)-O(2)-Pb(1)	112.3(4)
O(2)-Pb(2)-O(3)	81.6(6)	Pb(2)-O(2)-Pb(3)	106.1(5)
O(2)#1-Pb(3)-O(2)#5	117.2(5)	Pb(1)-O(2)-Pb(3)	100.0(4)
O(2)-Pb(4)-O(2)#5	71.1(5)	Pb(2)-O(2)-Pb(4)	102.0(4)
O(2)#3-Pb(4)-O(2)#5	113.8(5)	Pb(1)-O(2)-Pb(4)	126.6(5)
O(2)#7-Pb(4)-O(2)#5	74.2(5)	Pb(3)-O(2)-Pb(4)	108.6(4)
O(2)#1-Pb(3)-O(2)#6	71.6(5)	B(1)-O(1)-Pb(1)	134.0(2)
O(2)#5-Pb(3)-O(2)#6	76.9(5)	O(4)#10-N(1)-O(4)	122.0(6)
O(2)#1-Pb(3)-O(2)	76.9(5)	O(4)#10-N(1)-O(5)	119.0(3)
O(2)#5-Pb(3)-O(2)	71.6(5)	O(4)-N(1)-O(5)	119.0(3)
O(2)#6-Pb(3)-O(2)	117.2(5)	O(3)#9-B(1)-O(1)#2	118.1(19)
O(2)#7-Pb(4)-O(2)	113.8(5)	O(3)#9-B(1)-O(1)	118.1(19)
O(2)#7-Pb(4)-O(2)#3	71.1(5)	O(1)#2-B(1)-O(1)	124.0(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, y, z; #2 -x+1/2, -y+3/2, z; #3 -x-1/2, y, z; #4 x-1, y, z; #5 x, -y+1/2, z; #6 -x+1/2, -y+1/2, z; #7 -x-1/2, -y+1/2, z; #8 x+1, y, z; #9 -x, -y+1, -z+1; #10 -x-1/2, -y+3/2, z. **Table S3.** Bond Distances (Å) and angles [°] for H[Pb<sub>6</sub>( $\mu_3$ -O)<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub>.

Pb(1)-O(2)	2.305(11)	O(6)-Pb(1)#2	3.01(2)
Pb(1)-O(2)#1	2.323(11)	O(7)-Pb(1)#13	3.009(4)
Pb(1)-O(3)	2.343(12)	O(2)-Pb(1)#1	2.323(11)
Pb(1)-O(4)	2.985(13)	O(5)-Pb(1)#12	3.094(15)
Pb(1)-O(6)#2	3.01(2)	O(8)-Pb(2)#14	2.867(13)
Pb(1)-O(7)	3.009(4)	O(4)-Pb(2)#10	3.061(12)
Pb(1)-O(5)#3	3.094(15)	O(5)-Pb(2)#11	3.057(15)
Pb(2)-O(9)	2.261(10)	O(5)-Pb(2)#10	3.114(16)
Pb(2)-O(1)	2.281(10)	O(8)-Pb(3)#15	3.010(12)
Pb(2)-O(3)	2.368(11)	O(1)-Pb(3)#10	2.256(10)
Pb(2)-O(8)#5	2.867(13)	O(9)-Pb(3)#7	2.382(10)
Pb(2)-O(5)#6	3.057(15)	O(1)-B(1)	1.45(2)
Pb(2)-O(4)#4	3.061(12)	O(2)-B(1)	1.35(2)
Pb(2)-O(2)	3.082(11)	O(3)-B(1)#4	1.342(19)
Pb(2)-O(5)#4	3.114(16)	O(4)-N(1)	1.25(2)
Pb(3)-O(1)#4	2.256(10)	O(5)-N(1)	1.26(2)
Pb(3)-O(9)	2.320(10)	O(6)-N(1)	1.16(2)
Pb(3)-O(9)#7	2.382(10)	O(7)-N(2)	1.27(2)
Pb(3)-O(3)	2.833(13)	O(8)-N(2)	1.231(15)
Pb(3)-O(8)#8	3.010(12)	O(8)#13-N(2)	1.231(15)
O(2)-Pb(1)-O(2)#1	72.2(4)	O(6)#2-Pb(1)-O(5)#3	80.9(5)
O(2)-Pb(1)-O(3)	82.2(4)	O(7)-Pb(1)-O(5)#3	66.9(4)
O(2)#1-Pb(1)-O(3)	96.8(4)	O(1)#4-Pb(3)-O(9)	91.9(4)
O(2)-Pb(1)-O(4)	86.1(4)	O(1)#4-Pb(3)-O(9)#7	81.0(4)
O(2)#1-Pb(1)-O(4)	158.3(4)	O(9)-Pb(3)-O(9)#7	79.1(4)
O(3)-Pb(1)-O(4)	78.8(4)	O(1)#4-Pb(3)-O(3)	52.8(4)
O(2)-Pb(1)-O(6)#2	149.8(5)	O(9)-Pb(3)-O(3)	70.3(3)
O(2)#1-Pb(1)-O(6)#2	117.7(6)	O(9)#7-Pb(3)-O(3)	121.6(4)
O(3)-Pb(1)-O(6)#2	68.7(5)	O(1)#4-Pb(3)-O(8)#8	68.0(4)
O(4)-Pb(1)-O(6)#2	80.7(6)	O(9)-Pb(3)-O(8)#8	150.3(4)
O(2)-Pb(1)-O(7)	74.4(4)	O(9)#7-Pb(3)-O(8)#8	76.3(4)
O(2)#1-Pb(1)-O(7)	91.2(3)	O(3)-Pb(3)-O(8)#8	109.5(3)
O(3)-Pb(1)-O(7)	151.7(3)	O(4)-N(1)-O(5)	117.5(16)
O(4)-Pb(1)-O(7)	83.8(2)	O(6)-N(1)-O(4)	124(2)
O(6)#2-Pb(1)-O(7)	130.2(5)	O(6)-N(1)-O(5)	118(2)
O(2)-Pb(1)-O(5)#3	128.9(4)	O(8)-N(2)-O(8)#13	121(2)

O(2)#1-Pb(1)-O(5)#3	76.4(4)	O(8)-N(2)-O(7)	119.5(11)
O(3)-Pb(1)-O(5)#3	141.4(4)	O(8)#13-N(2)-O(7)	119.5(11)
O(4)-Pb(1)-O(5)#3	120.1(4)	O(3)#10-B(1)-O(2)	131.9(17)
Pb(1)-O(3)-Pb(2)	115.9(4)	O(3)#10-B(1)-O(1)	112.7(15)
O(9)-Pb(2)-O(1)	82.1(4)	O(2)-B(1)-O(1)	115.1(14)
O(9)-Pb(2)-O(3)	80.6(4)	Pb(3)#10-O(1)-Pb(2)	130.7(5)
O(1)-Pb(2)-O(3)	91.9(4)	B(1)-O(2)-Pb(1)	120.0(10)
O(9)-Pb(2)-O(8)#5	81.1(4)	B(1)-O(2)-Pb(1)#1	132.0(10)
O(1)-Pb(2)-O(8)#5	70.5(4)	Pb(1)-O(2)-Pb(1)#1	107.8(4)
O(3)-Pb(2)-O(8)#5	156.2(4)	B(1)-O(2)-Pb(2)	79.8(9)
O(9)-Pb(2)-O(5)#6	150.2(4)	Pb(1)-O(2)-Pb(2)	94.6(3)
O(1)-Pb(2)-O(5)#6	81.1(5)	Pb(1)#1-O(2)-Pb(2)	102.3(4)
O(3)-Pb(2)-O(5)#6	124.4(4)	B(1)#4-O(3)-Pb(1)	121.6(11)
O(8)#5-Pb(2)-O(5)#6	70.1(4)	B(1)#4-O(3)-Pb(2)	115.6(11)
O(9)-Pb(2)-O(4)#4	77.5(4)	B(1)#4-O(3)-Pb(3)	85.0(10)
O(1)-Pb(2)-O(4)#4	159.6(4)	Pb(1)-O(3)-Pb(3)	115.5(4)
O(3)-Pb(2)-O(4)#4	86.1(4)	Pb(2)-O(3)-Pb(3)	94.9(4)
O(8)#5-Pb(2)-O(4)#4	104.6(4)	N(1)-O(4)-Pb(1)	116.0(11)
O(5)#6-Pb(2)-O(4)#4	116.6(4)	N(1)-O(4)-Pb(2)#10	99.5(10)
O(9)-Pb(2)-O(2)	117.6(3)	Pb(1)-O(4)-Pb(2)#10	98.0(4)
O(6)-N(1)-O(4)	124(2)	N(1)-O(5)-Pb(2)#11	117.7(13)
O(6)-N(1)-O(5)	118(2)	N(1)-O(5)-Pb(1)#12	116.8(12)
O(1)-Pb(2)-O(2)	49.5(3)	Pb(2)#11-O(5)-Pb(1)#12	87.1(4)
O(3)-Pb(2)-O(2)	66.8(3)	N(1)-O(5)-Pb(2)#10	96.9(11)
O(8)#5-Pb(2)-O(2)	109.3(3)	Pb(2)#11-O(5)-Pb(2)#10	88.3(4)
O(5)#6-Pb(2)-O(2)	67.4(4)	Pb(1)#12-O(5)-Pb(2)#10	144.0(6)
O(4)#4-Pb(2)-O(2)	144.5(3)	N(1)-O(6)-Pb(1)#2	157(2)
O(9)-Pb(2)-O(5)#4	83.1(4)	N(2)-O(7)-Pb(1)#13	102.2(3)
O(1)-Pb(2)-O(5)#4	135.4(4)	N(2)-O(7)-Pb(1)	102.2(3)
O(3)-Pb(2)-O(5)#4	126.6(4)	Pb(1)#13-O(7)-Pb(1)	155.7(6)
O(8)#5-Pb(2)-O(5)#4	65.7(4)	N(2)-O(8)-Pb(2)#14	124.2(9)
O(5)#6-Pb(2)-O(5)#4	91.7(4)	N(2)-O(8)-Pb(3)#15	127.7(10)
O(4)#4-Pb(2)-O(5)#4	40.7(4)	Pb(2)#14-O(8)-Pb(3)#15	89.1(3)
O(2)-Pb(2)-O(5)#4	158.4(4)	Pb(2)-O(9)-Pb(3)	114.2(4)
Pb(3)-O(9)-Pb(3)#7	100.9(4)	Pb(2)-O(9)-Pb(3)#7	118.1(4)

Symmetry transformations used to generate equivalent atoms:#1 -x, -y, -z; #2 -x+1/2, -y+1/2, -z; #3 x-1/2, -y+1/2, z-1/2; #4 x, -y, z-1/2; #5 x+1/2, y-1/2, z; #6 -x+1/2, y-1/2, -z+1/2; #7 -x+1, -y, -z; #8 x+1/2, -y+1/2, z-1/2; #9 -x+1, y, -z+1/2 #10 x, -y, z+1/2 #11 -x+1/2, y+1/2, -z+1/2; #12 x+1/2, -y+1/2, z+1/2; #13 -x, y, -z+1/2; #14 x-1/2, y+1/2, z; #15 x-1/2, -y+1/2, z+1/2.

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Pb(1)-O(11)#1	2.362(6)	Pb(7)-O(16)#5	2.567(5)
Pb(1)-O(12)	2.365(5)	Pb(7)-O(14)#4	2.574(5)
Pb(1)-O(11)	2.379(5)	Pb(7)-O(2)#7	3.092(8)
Pb(1)-O(10)	2.602(5)	Pb(7)-O(3)#7	3.060(7)
Pb(1)-O(1)#4	2.977(7)	Pb(7)-O(7)	3.049(9)
Pb(2)-O(11)	2.227(5)	Pb(7)-O(17)	2.748(6)
Pb(2)-O(18)#2	2.331(6)	Pb(8)-O(18)	2.288(5)
Pb(2)-O(10)	2.402(5)	Pb(8)-O(17)	2.171(5)
Pb(2)-O(15)#1	2.629(6)	Pb(8)-O(16)	2.256(6)
Pb(2)-O(2)#10	3.034(6)	N(3)-O(7)	1.220(11)
Pb(3)-O(12)	2.210(5)	N(3)-O(8)	1.230(13)
Pb(3)-O(11)#1	2.341(6)	N(3)-O(9)	1.239(10)
Pb(3)-O(15)	2.578(6)	O(1)-N(1)	1.206(9)
Pb(3)-O(13)#3	2.640(5)	O(2)-N(1)	1.265(9)
Pb(3)-O(6) #1	2.937(7)	O(3)-N(1)	1.247(9)
Pb(3)-O(9) #7	3.071(7)	O(4)-N(2)	1.259(10)
Pb(4)-O(14)	2.237(6)	O(5)-N(2)	1.273(9)
Pb(4)-O(15)	2.260(5)	O(6)-N(2)	1.249(10)
Pb(4)-O(13)#3	2.393(5)	O(10)-B(1)	1.410(11)
Pb(4)-O(5) #9	2.800(6)	O(13)-B(1)	1.390(10)
Pb(4)-O(2) #8	2.973(6)	O(17)-B(1)#6	1.359(12)
Pb(4)-O(1) #3	3.067(7)	O(15)-B(2)	1.369(11)
Pb(5)-O(12)	2.328(5)	O(18)-B(2)#5	1.403(11)
Pb(5)-O(12)#3	2.337(5)	O(19)-B(2)	1.356(13)
Pb(5)-O(13)	2.408(6)	B(1)-O(17)#2	1.359(12)
Pb(5)-O(10)	2.519(6)	B(2)-O(18)#5	1.403(11)
Pb(5)-O(6)#1	2.890(8)	O(11)-Pb(3)#1	2.341(6)
Pb(5)-O(9)#7	3.094(6)	O(11)-Pb(1)#1	2.362(6)
Pb(6)-O(14)	2.250(5)	O(12)-Pb(5)#3	2.337(5)
Pb(6)-O(14)#4	2.266(6)	O(13)-Pb(4)#3	2.393(5)
Pb(6)-O(19)	2.299(5)	O(13)-Pb(3)#3	2.640(5)
Pb(6)-O(7)	2.963(8)	O(14)-Pb(6)#4	2.266(6)
Pb(6)-O(17)#4	2.919(5)	O(14)-Pb(7)#4	2.574(5)
Pb(7)-O(19)	2.367(6)	O(15)-Pb(2)#1	2.629(6)
Pb(7)-O(16)	2.426(6)	O(16)-Pb(7)#5	2.567(5)
O(11)#1-Pb(1)-O(12)	75.61(18)	O(14)-Pb(6)-O(14)#4	77.8(2)
O(11)#1-Pb(1)-O(11)	75.4(2)	O(14)-Pb(6)-O(19)	85.7(2)
O(12)-Pb(1)-O(11)	116.72(19)	O(14)#4-Pb(6)-O(19)	77.8(2)
O(11)#1-Pb(1)-O(10)	118.22(19)	O(19)-Pb(7)-O(14)#4	70.82(18)
O(12)-Pb(1)-O(10)	71.74(19)	O(16)-Pb(7)-O(14)#4	104.67(17)

**Table S4.** Bond Distances (Å) and angles [°] for H[Pb<sub>8</sub>( $\mu_4$ -O)<sub>3</sub>( $\mu_3$ -O)(BO<sub>3</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3.</sub>

O(11)-Pb(1)-O(10)	74.85(16)	O(16)#5-Pb(7)-O(14)#4	152.20(18)
O(11)-Pb(2)-O(18)#2	92.2(2)	O(19)-Pb(7)-O(17)	116.78(19)
O(11)-Pb(2)-O(10)	81.75(18)	O(16)-Pb(7)-O(17)	65.69(19)
O(18)#2-Pb(2)-O(10)	78.33(19)	O(14)#4-Pb(7)-O(17)	68.97(16)
O(11)-Pb(2)-O(15)#1	78.67(19)	O(17)-Pb(8)-O(16)	79.1(2)
O(18)#2-Pb(2)-O(15)#1	55.58(17)	O(17)-Pb(8)-O(18)	79.9(2)
O(10)-Pb(2)-O(15)#1	128.49(19)	O(16)-Pb(8)-O(18)	79.0(2)
O(12)-Pb(3)-O(11)#1	79.01(19)	O(7)-N(3)-O(8)	116.3(10)
O(12)-Pb(3)-O(15)	113.97(19)	O(7)-N(3)-O(9)	122.8(10)
O(11)#1-Pb(3)-O(15)	77.75(19)	O(8)-N(3)-O(9)	120.9(10)
O(12)-Pb(3)-O(13)#3	74.18(19)	Pb(3)-O(12)-Pb(1)	104.63(18)
O(11)#1-Pb(3)-O(13)#3	120.87(18)	Pb(5)-O(12)-Pb(1)	113.5(2)
O(15)-Pb(3)-O(13)#3	67.28(16)	Pb(5)#3-O(12)-Pb(1)	112.2(2)
O(14)-Pb(4)-O(15)	92.2(2)	B(1)-O(13)-Pb(4)#3	118.9(5)
O(14)-Pb(4)-O(13)#3	90.0(2)	B(1)-O(13)-Pb(5)	96.2(5)
O(15)-Pb(4)-O(13)#3	76.79(18)	Pb(4)#3-O(13)-Pb(5)	115.8(2)
O(12)-Pb(5)-O(12)#3	76.04(18)	B(1)-O(13)-Pb(3)#3	122.3(5)
O(12)-Pb(5)-O(13)	110.65(19)	Pb(4)#3-O(13)-Pb(3)#3	104.78(17)
O(12)#3-Pb(5)-O(13)	76.72(19)	Pb(5)-O(13)-Pb(3)#3	96.7(2)
O(12)-Pb(5)-O(10)	73.87(19)	Pb(4)-O(14)-Pb(6)	116.4(2)
O(12)#3-Pb(5)-O(10)	108.69(19)	Pb(4)-O(14)-Pb(6)#4	124.3(2)
O(13)-Pb(5)-O(10)	57.35(17)	Pb(6)-O(14)-Pb(6)#4	102.2(2)
O(16)#5-Pb(7)-O(17)	132.05(16)	Pb(4)-O(14)-Pb(7)#4	106.04(19)
Pb(2)-O(10)-Pb(1)	95.74(16)	Pb(6)-O(14)-Pb(7)#4	106.7(2)
Pb(5)-O(10)-Pb(1)	100.1(2)	Pb(6)#4-O(14)-Pb(7)#4	98.8(2)
Pb(2)-O(11)-Pb(3)#1	110.8(2)	B(2)-O(15)-Pb(4)	128.5(6)
Pb(2)-O(11)-Pb(1)#1	113.9(2)	B(2)-O(15)-Pb(3)	101.3(5)
Pb(3)#1-O(11)-Pb(1)#1	100.72(18)	Pb(4)-O(15)-Pb(3)	110.97(19)
Pb(2)-O(11)-Pb(1)	107.42(19)	B(2)-O(15)-Pb(2)#1	88.8(5)
Pb(3)#1-O(11)-Pb(1)	119.3(2)	Pb(4)-O(15)-Pb(2)#1	127.0(3)
Pb(1)#1-O(11)-Pb(1)	104.6(2)	Pb(3)-O(15)-Pb(2)#1	92.50(19)
Pb(3)-O(12)-Pb(5)	110.6(2)	Pb(8)-O(16)-Pb(7)	102.3(2)
Pb(3)-O(12)-Pb(5)#3	112.2(2)	Pb(8)-O(16)-Pb(7)#5	115.4(2)
Pb(5)-O(12)-Pb(5)#3	103.96(18)	Pb(7)-O(16)-Pb(7)#5	103.93(19)
O(17)#2-B(1)-O(13)	121.1(8)	B(1)#6-O(17)-Pb(8)	121.6(5)
O(17)#2-B(1)-O(10)	123.5(7)	B(1)#6-O(17)-Pb(7)	108.9(5)
O(13)-B(1)-O(10)	115.4(8)	Pb(8)-O(17)-Pb(7)	95.0(2)
O(6)-N(2)-O(4)	120.8(8)	B(2)#5-O(18)-Pb(8)	117.8(6)
O(6)-N(2)-O(5)	120.4(8)	B(2)#5-O(18)-Pb(2)#6	100.9(5)
O(4)-N(2)-O(5)	118.7(8)	Pb(8)-O(18)-Pb(2)#6	127.2(3)
O(19)-B(2)-O(15)	125.3(8)	B(2)-O(19)-Pb(6)	122.3(5)
O(19)-B(2)-O(18)#5	120.1(8)	B(2)-O(19)-Pb(7)	132.0(5)
O(15)-B(2)-O(18)#5	114.2(9)	Pb(6)-O(19)-Pb(7)	104.2(2)

O(1)-N(1)-O(3)	120.1(7)	O(3)-N(1)-O(2)	118.4(8)
O(1)-N(1)-O(2)	121.4(8)		

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



Chart S1. The products obtained at different reaction condition.



Chart S2. Molar ratio of Pb<sup>2+</sup>/(BO<sub>2</sub>)<sup>-</sup> under different pH Values.



**Figure S1.** Experimental and calculated powder X-ray diffraction patterns of  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$  (a),  $H[Pb_6(\mu_3-O)_2(BO_3)_2](NO_3)_3$  (b) and  $H[Pb_8(\mu_4-O)_3(\mu_3-O)(BO_3)_2](NO_3)_3$  (c),  $Pb_2(BO_3)(NO_3)$  (d) and  $Pb_4(NO_3)_4(OH)_4$  (e).



Figure S2. UV-vis-NIR absorption spectra of  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$  (a),  $H[Pb_6(\mu_3-D)_4(BO_3)](NO_3)$  (b),  $H[Pb_6(\mu_3-D)_4(BO_3)](NO_3)$  (b),  $H[Pb_6(\mu_3-D)_4(BO_3)](NO_3)$  (c),  $H[Pb_6(\mu_3-D)_4(BO_3)$ 

 $O_{2}(BO_{3})_{2}[NO_{3})_{3}(\mathbf{b})$  and  $H[Pb_{8}(\mu_{4}-O_{3}(\mu_{3}-O)(BO_{3})_{2}](NO_{3})_{3}(\mathbf{c}).$ 



Figure S3. IR spectra of  $[Pb_6(\mu_4-O)_4(BO_3)](NO_3)$  (a),  $H[Pb_6(\mu_3-O)_2(BO_3)_2](NO_3)_3$ (b) and  $H[Pb_8(\mu_4-O)_3(\mu_3-O)(BO_3)_2](NO_3)_3$  (c).