Supporting Information

Synthesis and optical properties of the first lead borate bromide with isolated BO_3 groups: $Pb_2Ba_3(BO_3)_3Br$

Qun Jing[1,2], Xiaoyu Dong[1,3], Zhihua Yang[1*], Shilie Pan[1*]

[1] Key Laboratory of Functional Materials and Devices for Special Environments of CAS, Xinjiang Technical Institute of Physics & Chemistry of CAS, Xinjiang Key Laboratory of Electronic Information Materials and Devices, 40-1 South Beijing Road, Urumqi 830011, China

[2] Department of Physics, School of Science, Shihezi University, Shihezi 832000, China

[3] Engineering Department of Chemistry and Environment, Xinjiang Institute of Engineering; 236 Nanchang Road, Urumqi 830091, China;

*To whom correspondence should be addressed

E-mail: zhyang@ms.xjb.ac.cn (Zhihua Yang) Tel: (86)-991-3810816. Fax: (86)991-3838957.

E-mail: slpan@ms.xjb.ac.cn (Shilie Pan) Tel: (86)-991-3674558. Fax: (86)991-3838957

Table S1. Bond lengths [Å] and angles [deg.] for $Pb_2Ba_3(BO_3)_3Br$.

Pb(1)-O(5)	2.319(8)
Pb(1)-O(1)	2.360(8)
Pb(1)-O(4)	2.474(7)
Pb(1)-Br(1)	3.1720(7)
Ba(1)-O(3)	2.608(11)
Ba(1)-O(5)#3	2.796(9)
Ba(1)-O(5)#4	2.796(9)
Ba(1)-O(2)#5	2.836(8)
Ba(1)-O(2)#6	2.836(8)
Ba(1)-O(4)#3	2.947(7)
Ba(1)-O(4)#4	2.947(7)
Ba(1)-Br(1)#2	3.4412(11)
Ba(1)-Br(1)#7	3.4412(11)
Ba(2)-O(1)#3	2.666(9)
Ba(2)-O(1)	2.666(9)
Ba(2)-O(2)#8	2.812(9)
Ba(2)-O(2)#6	2.812(9)
Ba(2)-O(3)	2.9243(8)
Ba(2)-O(3)#2	2.9243(8)
Ba(2)-O(4)	2.929(8)
Ba(2)-O(4)#3	2.929(8)
Ba(3)-O(2)	2.737(9)
Ba(3)-O(2)#8	2.737(9)
Ba(3)-O(1)#9	2.804(9)
Ba(3)-O(1)#3	2.804(9)
Ba(3)-O(3)#2	2.9460(9)
Ba(3)-O(3)#9	2.9460(9)
Ba(3)-O(4)#5	3.047(7)
Ba(3)-O(4)#2	3.047(7)
Ba(3)-O(5)#10	3.190(9)
Ba(3)-O(5)#11	3.190(9)
B(1)-O(4)#12	1.390(11)
B(1)-O(4)	1.390(11)

B(1)-O(3)	1.40(2)
B(2)-O(2)#8	1.367(15)
B(2)-O(5)	1.370(15)
B(2)-O(1)#11	1.387(15)
O(5)-Pb(1)-O(1)	99.3(3)
O(5)-Pb(1)-O(4)	89.5(3)
O(1)-Pb(1)-O(4)	76.6(3)
O(3)-Ba(1)-O(5)#3	112.9(2)
O(3)-Ba(1)-O(5)#4	112.9(2)
O(5)#3-Ba(1)-O(5)#4	134.3(4)
O(3)-Ba(1)-O(2)#5	70.94(16)
O(5)#3-Ba(1)-O(2)#5	154.1(3)
O(5)#4-Ba(1)-O(2)#5	49.8(2)
O(3)-Ba(1)-O(2)#6	70.94(16)
O(5)#3-Ba(1)-O(2)#6	49.8(2)
O(5)#4-Ba(1)-O(2)#6	154.1(3)
O(2)#5-Ba(1)-O(2)#6	141.9(3)
O(3)-Ba(1)-O(4)#3	74.42(15)
O(5)#3-Ba(1)-O(4)#3	71.9(2)
O(5)#4-Ba(1)-O(4)#3	121.3(2)
O(2)#5-Ba(1)-O(4)#3	85.3(2)
O(2)#6-Ba(1)-O(4)#3	84.6(3)
O(3)-Ba(1)-O(4)#4	74.42(15)
O(5)#3-Ba(1)-O(4)#4	121.3(2)
O(5)#4-Ba(1)-O(4)#4	71.9(2)
O(2)#5-Ba(1)-O(4)#4	84.6(3)
O(2)#6-Ba(1)-O(4)#4	85.3(2)
O(4)#3-Ba(1)-O(4)#4	148.8(3)
O(1)#3-Ba(2)-O(1)	148.0(3)
O(1)#3-Ba(2)-O(2)#8	79.5(2)
O(1)-Ba(2)-O(2)#8	94.0(2)
O(1)#3-Ba(2)-O(2)#6	94.0(2)
O(1)-Ba(2)-O(2)#6	79.5(2)
O(2)#8-Ba(2)-O(2)#6	156.4(3)

O(1)#3-Ba(2)-O(3)	132.2(3)
O(1)-Ba(2)-O(3)	74.0(2)
O(2)#8-Ba(2)-O(3)	133.4(2)
O(2)#6-Ba(2)-O(3)	66.9(2)
O(1)#3-Ba(2)-O(3)#2	74.0(2)
O(1)-Ba(2)-O(3)#2	132.2(3)
O(2)#8-Ba(2)-O(3)#2	66.9(2)
O(2)#6-Ba(2)-O(3)#2	133.4(2)
O(3)-Ba(2)-O(3)#2	87.97(3)
O(1)#3-Ba(2)-O(4)	144.3(2)
O(1)-Ba(2)-O(4)	64.6(2)
O(2)#8-Ba(2)-O(4)	85.4(2)
O(2)#6-Ba(2)-O(4)	111.4(2)
O(3)-Ba(2)-O(4)	48.5(2)
O(3)#2-Ba(2)-O(4)	70.3(2)
O(1)#3-Ba(2)-O(4)#3	64.6(2)
O(1)-Ba(2)-O(4)#3	144.3(2)
O(2)#8-Ba(2)-O(4)#3	111.4(2)
O(2)#6-Ba(2)-O(4)#3	85.4(2)
O(3)-Ba(2)-O(4)#3	70.3(2)
O(3)#2-Ba(2)-O(4)#3	48.5(2)
O(4)-Ba(2)-O(4)#3	91.9(3)
O(2)-Ba(3)-O(2)#8	157.0(3)
O(2)-Ba(3)-O(1)#9	78.4(2)
O(2)#8-Ba(3)-O(1)#9	95.8(2)
O(2)-Ba(3)-O(1)#3	95.8(2)
O(2)#8-Ba(3)-O(1)#3	78.4(2)
O(1)#9-Ba(3)-O(1)#3	150.9(3)
O(2)-Ba(3)-O(3)#2	132.1(3)
O(2)#8-Ba(3)-O(3)#2	67.6(2)
O(1)#9-Ba(3)-O(3)#2	132.7(2)
O(1)#3-Ba(3)-O(3)#2	71.7(2)
O(2)-Ba(3)-O(3)#9	67.6(2)
O(2)#8-Ba(3)-O(3)#9	132.1(3)

O(1)#9-Ba(3)-O(3)#9	71.7(2)
O(1)#3-Ba(3)-O(3)#9	132.7(2)
O(3)#2-Ba(3)-O(3)#9	87.16(3)
O(2)-Ba(3)-O(4)#5	111.9(2)
O(2)#8-Ba(3)-O(4)#5	85.1(2)
O(1)#9-Ba(3)-O(4)#5	66.2(2)
O(1)#3-Ba(3)-O(4)#5	140.1(2)
O(3)#2-Ba(3)-O(4)#5	68.4(2)
O(3)#9-Ba(3)-O(4)#5	47.2(2)
O(2)-Ba(3)-O(4)#2	85.1(2)
O(2)#8-Ba(3)-O(4)#2	111.9(2)
O(1)#9-Ba(3)-O(4)#2	140.1(2)
O(1)#3-Ba(3)-O(4)#2	66.2(2)
O(3)#2-Ba(3)-O(4)#2	47.2(2)
O(3)#9-Ba(3)-O(4)#2	68.4(2)
O(4)#5-Ba(3)-O(4)#2	87.4(3)
O(2)-Ba(3)-O(5)#10	74.3(2)
O(2)#8-Ba(3)-O(5)#10	86.1(2)
O(1)#9-Ba(3)-O(5)#10	105.6(2)
O(1)#3-Ba(3)-O(5)#10	46.0(2)
O(3)#2-Ba(3)-O(5)#10	116.37(18)
O(3)#9-Ba(3)-O(5)#10	141.6(2)
O(4)#5-Ba(3)-O(5)#10	167.2(2)
O(4)#2-Ba(3)-O(5)#10	104.5(2)
O(2)-Ba(3)-O(5)#11	86.1(2)
O(2)#8-Ba(3)-O(5)#11	74.3(2)
O(1)#9-Ba(3)-O(5)#11	46.0(2)
O(1)#3-Ba(3)-O(5)#11	105.6(2)
O(3)#2-Ba(3)-O(5)#11	141.6(2)
O(3)#9-Ba(3)-O(5)#11	116.37(18)
O(4)#5-Ba(3)-O(5)#11	104.5(2)
O(4)#2-Ba(3)-O(5)#11	167.2(2)
O(5)#10-Ba(3)-O(5)#11	64.1(3)
O(4)#12-B(1)-O(4)	122.4(14)

O(4)#12-B(1)-O(3)	118.8(7)
O(4)-B(1)-O(3)	118.8(7)
O(2)#8-B(2)-O(5)	120.0(11)
O(2)#8-B(2)-O(1)#11	121.6(11)
O(5)-B(2)-O(1)#11	118.4(11)

Symmetry transformations used to generate equivalent atoms:

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

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

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

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

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

#13 -x+2,y,-z+5/2 #14 x+1,y,z

Figure S1. The IR spectrum of $Pb_2Ba_3(BO_3)_3Br$.