Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters for Pb_2BO_3Br

atom	x	y	z	U(eq)
Pb(1)	3333	6667	2121(3)	13(1)
Br(1)	0	0	5000	30(2)
O(1)	2640(80)	2640(80)	0	32(11)
B(1)	0	10000	0	0(10)

Table S2. Bond lengths (Å) for Pb_2BO_3Br

Pb(1)-O(1)#1	2.34(2)	O(1)#1-Pb(1)-O(1)#2	86.6(5)
Pb(1)-O(1)	2.34(2)	O(1)-Pb(1)-O(1)#2	86.6(6)
Pb(1)-O(1)#2	2.34(2)	B(1)#3-O(1)-Pb(1)	120.1(8)
O(1)-B(1)#3	1.31(4)	B(1)#3-O(1)-Pb(1)#4	120.1(8)
O(1)-Pb(1)#4	2.34(2)	Pb(1)-O(1)-Pb(1)#4	119.8(17)
B(1)-O(1)#5	1.31(4)	O(1)#5-B(1)-O(1)#1	120.000(11)
B(1)-O(1)#1	1.31(4)	O(1)#5-B(1)-O(1)#6	120.000(1)
B(1)-O(1)#6	1.31(4)	O(1)#1-B(1)-O(1)#6	120.000(17)
O(1)#1-Pb(1)-O(1)	86.6(6)		

Symmetry transformations used to generate equivalent atoms:

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

#4 y, x,-z #5 x, y+1, z #6 -y, x-y+1, z

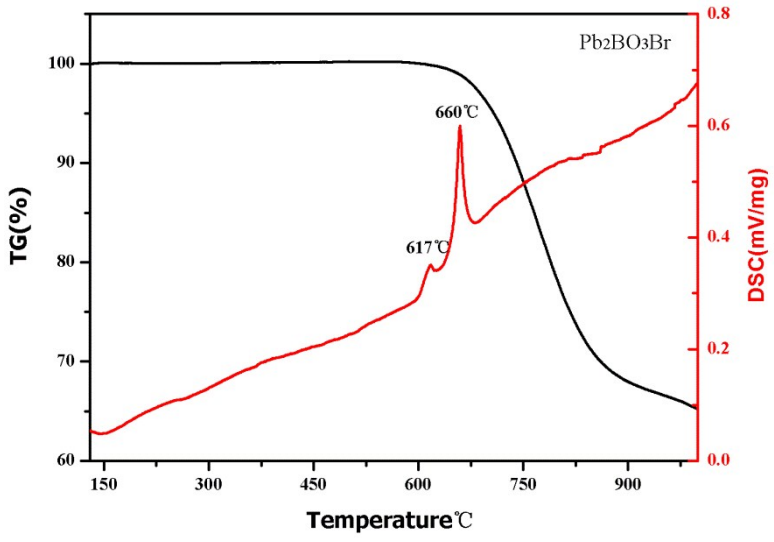

Fig.S1. TG and DSC curves of Pb_2BO_3Br

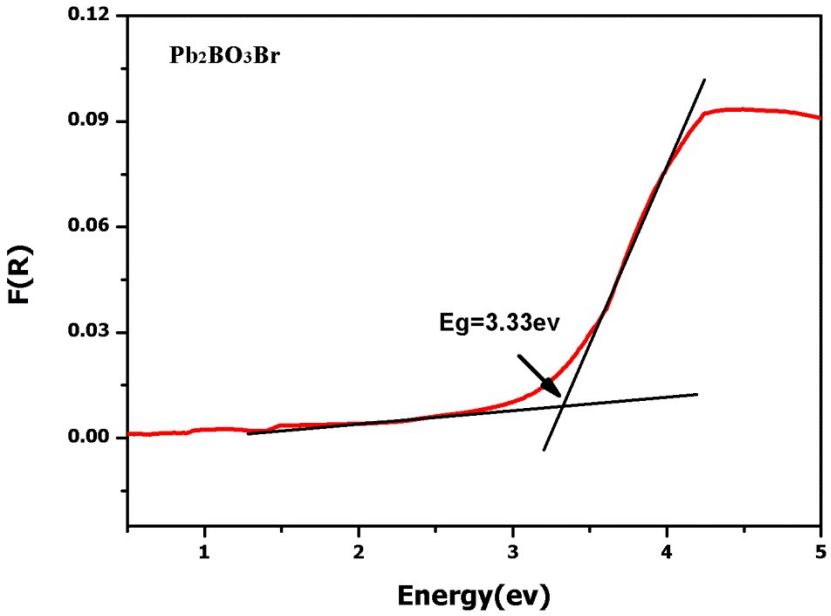

Fig. S2 Optical diffuse reflectance spectra for Pb_2BO_3Br