Electronic Supplementary Information (ESI)

Structural Insights for the Design of New Borate-phosphates: Synthesis, Crystal Structure and Optical Properties of $Pb_4O(BO_3)(PO_4)$ and $Bi_4O_3(BO_3)(PO_4)$

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Table S1. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $Pb_4O(BO_3)(PO_4)$ and $Bi_4O_3(BO_3)(PO_4)$.

Atom	*Wyck.*	x/*a*	y/*b*	z/*c*	U_{eq}[a]
		$Pb_4O(BO_3)(PO_4)$			
Pb(1)	4*e*	0.86999(9)	0.22743(11)	0.06858(7)	0.013(1)
Pb(2)	4*e*	0.45093(9)	0.19882(11)	0.07416(7)	0.016(1)
Pb(3)	4*e*	0.75925(10)	-	0.29334(7)	0.016(1)
Pb(4)	4*e*	0.76925(9)	0.49161(10)	0.26588(7)	0.014(1)
B(1)	4*e*	0.458(3)	0.730(3)	0.1345(18)	0.008(5)
P(1)	4*e*	0.8992(7)	-0.2502(7)	0.1018(5)	0.014(1)
O(1)	4*e*	0.7088(16)	0.2177(17)	0.1629(11)	0.012(3)
O(2)	4*e*	0.9342(18)	-0.140(2)	0.2120(12)	0.027(4)
O(3)	4*e*	1.0349(17)	-0.326(2)	0.0953(12)	0.023(3)
O(4)	4*e*	0.8278(16)	-0.1157(18)	0.0032(12)	0.020(3)
O(5)	4*e*	0.6854(17)	0.2497(16)	-0.1129(12)	0.014(3)
O(6)	4*e*	0.7937(15)	0.5859(18)	0.0881(11)	0.016(3)
O(7)	4*e*	0.5291(18)	0.589(2)	0.2056(16)	0.036(4)
O(8)	4*e*	0.4729(17)	0.133(2)	-0.0971(11)	0.023(4)
		$Bi_4O_3(BO_3)(PO_4)$			
Bi(1)	8*c*	0.05342(10)	0.71229(4)	0.30675(2)	0.013(1)
Bi(2)	8*c*	0.54041(11)	0.52313(4)	0.30828(3)	0.017(1)
Bi(3)	8*c*	0.03571(10)	0.54061(4)	0.42524(2)	0.012(1)
Bi(4)	8*c*	0.56453(10)	0.73778(4)	0.41555(3)	0.016(1)
B(1)	8*c*	0.537(3)	0.3862(12)	0.1878(8)	0.015(4)
P(1)	8*c*	0.0091(7)	0.8760(3)	0.45401(18)	0.013(1)
O(1)	8*c*	0.2619(18)	0.6271(6)	0.3697(4)	0.013(2)
O(2)	8*c*	0.2979(18)	0.6189(6)	0.2494(4)	0.011(2)
O(3)	8*c*	0.7719(18)	0.6332(6)	0.3697(4)	0.014(2)
O(4)	8*c*	-0.0383(18)	0.7913(7)	0.4121(5)	0.018(2)
O(5)	8*c*	0.207(2)	0.8511(7)	0.4980(5)	0.022(3)
O(6)	8*c*	0.093(2)	0.9607(8)	0.4163(5)	0.026(3)
O(7)	8*c*	-0.232(2)	0.8930(8)	0.4853(5)	0.030(3)
O(8)	8*c*	0.698(2)	0.4201(8)	0.2286(6)	0.031(3)
O(9)	8*c*	-0.074(2)	0.4414(9)	0.3534(5)	0.030(3)
O(10)	8*c*	0.480(2)	0.7866(9)	0.3195(6)	0.029(3)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected Bond Distances (Å) for the two compounds.

		$Pb_4O(BO_3)(PO_4)$	
Pb(1)-O(5)	2.368(15)	Pb(4)-O(1)	2.278(12)
Pb(1)-O(1)	2.401(13)	Pb(4)-O(7)	2.362(16)
Pb(1)-O(4)	2.528(13)	Pb(4)-O(6)	2.495(13)
Pb(1)-O(6)	2.670(13)	Pb(4)-O(5)	2.663(13)
Pb(1)-O(3)	2.741(14)	Pb(4)-O(2)	3.300(16)
Pb(1)-O(2)	3.088(14)	Pb(4)-O(2)	3.067(18)
Pb(1)-O(2)	2.908(13)	Pb(4)-O(3)	3.058(13)
		Pb(4)-O(4)	3.013(15)
Pb(2)-O(8)	2.354(13)		
Pb(2)-O(1)	2.427(15)	B(1)-O(7)	1.350(3)
Pb(2)-O(8)	2.434(15)	B(1)-O(5)	1.380(3)
Pb(2)-O(4)	2.683(15)	B(1)-O(8)	1.390(3)
Pb(2)-O(6)	2.966(12)		
Pb(2)-O(7)	3.151(11)	P(1)-O(3)	1.515(16)
Pb(2)-O(7)	2.877(21)	P(1)-O(4)	1.521(15)
		P(1)-O(2)	1.535(14)
Pb(3)-O(1)	2.225(12)	P(1)-O(6)	1.536(14)
Pb(3)-O(3)	2.400(16)		
Pb(3)-O(5)	2.460(13)		
Pb(3)-O(2)	2.568(14)		
Pb(3)-O(7)	3.026(19)		
Pb(3)-O(8)	2.844(12)		
		$Bi_4O_3(BO_3)(PO_4)$	
Bi(1)-O(1)	2.191(10)	Bi(3)-O(5)	3.447(10)
Bi(1)-O(2)	2.291(10)	Bi(3)-O(7)	3.001(11)
Bi(1)-O(2)	2.312(10)		
Bi(1)-O(3)	2.387(10)	Bi(4)-O(3)	2.138(10)
Bi(1)-O(10)	2.597(13)	Bi(4)-O(4)	2.326(11)
Bi(1)-O(4)	2.680(11)	Bi(4)-O(10)	2.327(13)
Bi(1)-O(8)	3.335(11)	Bi(4)-O(5)	2.453(11)
Bi(1)-O(10)	3.355(11)	Bi(4)-O(1)	2.515(10)
Bi(1)-O(10)	3.069(13)	Bi(4)-O(4)	3.422(10)
		Bi(4)-O(5)	3.154(10)
Bi(2)-O(2)	2.325(10)	Bi(4)-O(7)	2.924(11)
Bi(2)-O(2)#3	2.357(10)	Bi(4)-O(7)	3.336(11)
Bi(2)-O(3)	2.445(10)	Bi(4)-O(9)	3.198(12)
Bi(2)-O(8)	2.474(12)		
Bi(2)-O(8)	2.530(12)	B(1)-O(9)	1.360(2)
Bi(2)-O(1)	2.540(10)	B(1)-O(8)	1.370(2)
Bi(2)-O(9)	2.632(12)	B(1)-O(10)	1.420(2)
Bi(2)-O(6)	2.700(12)		
		P(1)-O(5)	1.519(11)
Bi(3)-O(1)	2.153(10)	P(1)-O(7)	1.527(13)
Bi(3)-O(9)	2.229(12)	P(1)-O(6)	1.539(12)
Bi(3)-O(3)	2.328(10)	P(1)-O(4)	1.547(11)

Bi(3)-O(6)	2.353(11)
Bi(3)-O(7)	2.575(13)
Bi(3)-O(5)	2.942(11)

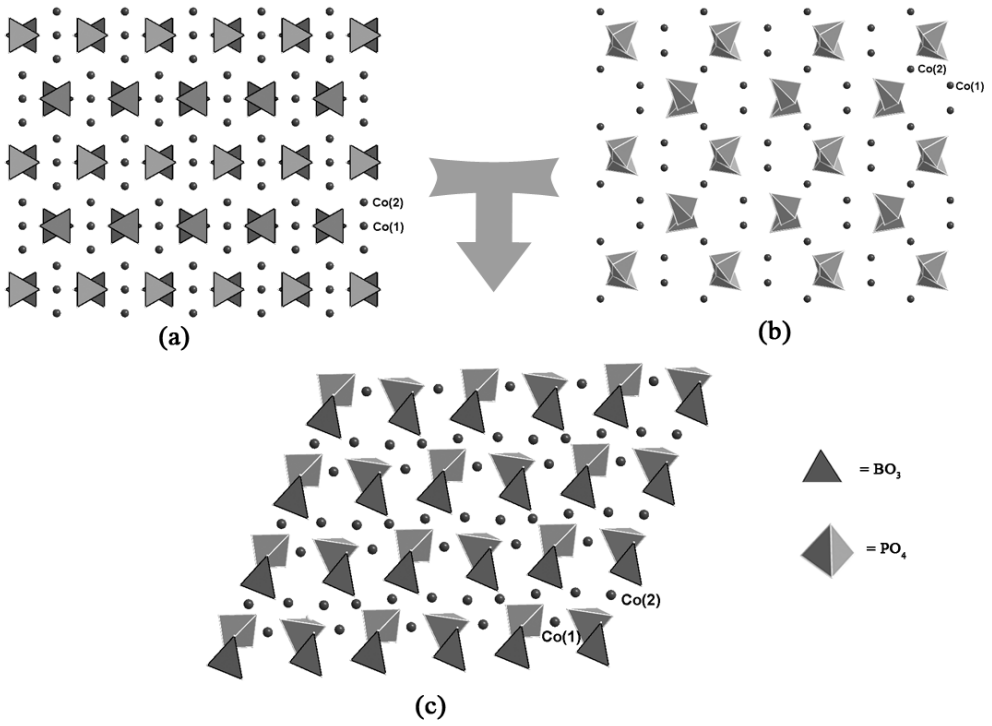

Fig. S1 View of crystal structure of (a) $Co_3(BO_3)_2$, (b) $Co_3(PO_4)_2$, and (c) $Co_3(BO_3)(PO_4)$;

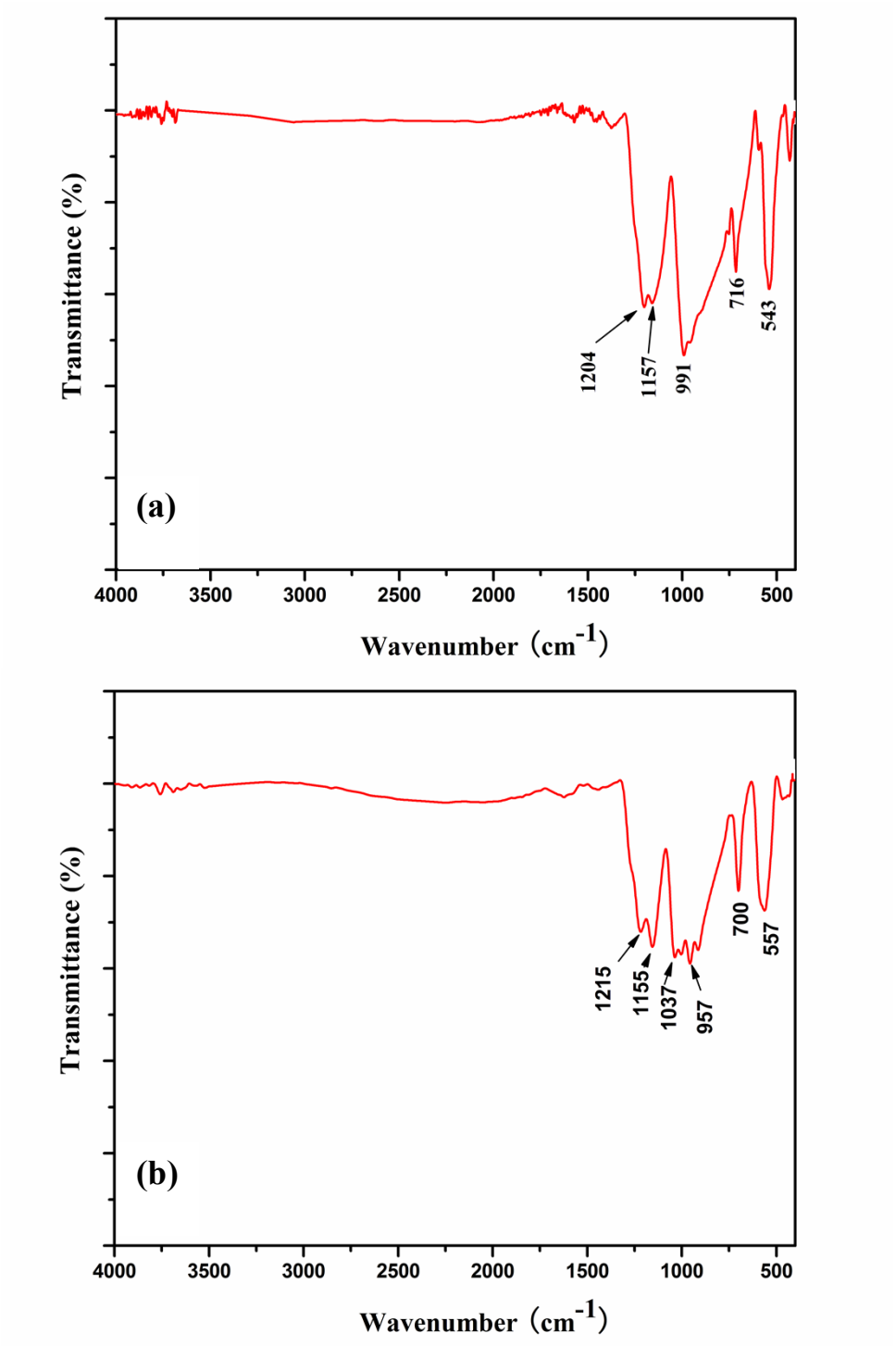

Fig. S2 IR Spectroscopy for (a) $Pb_4O(BO_3)(PO_4)$ and (b) $Bi_4O_3(BO_3)(PO_4)$.

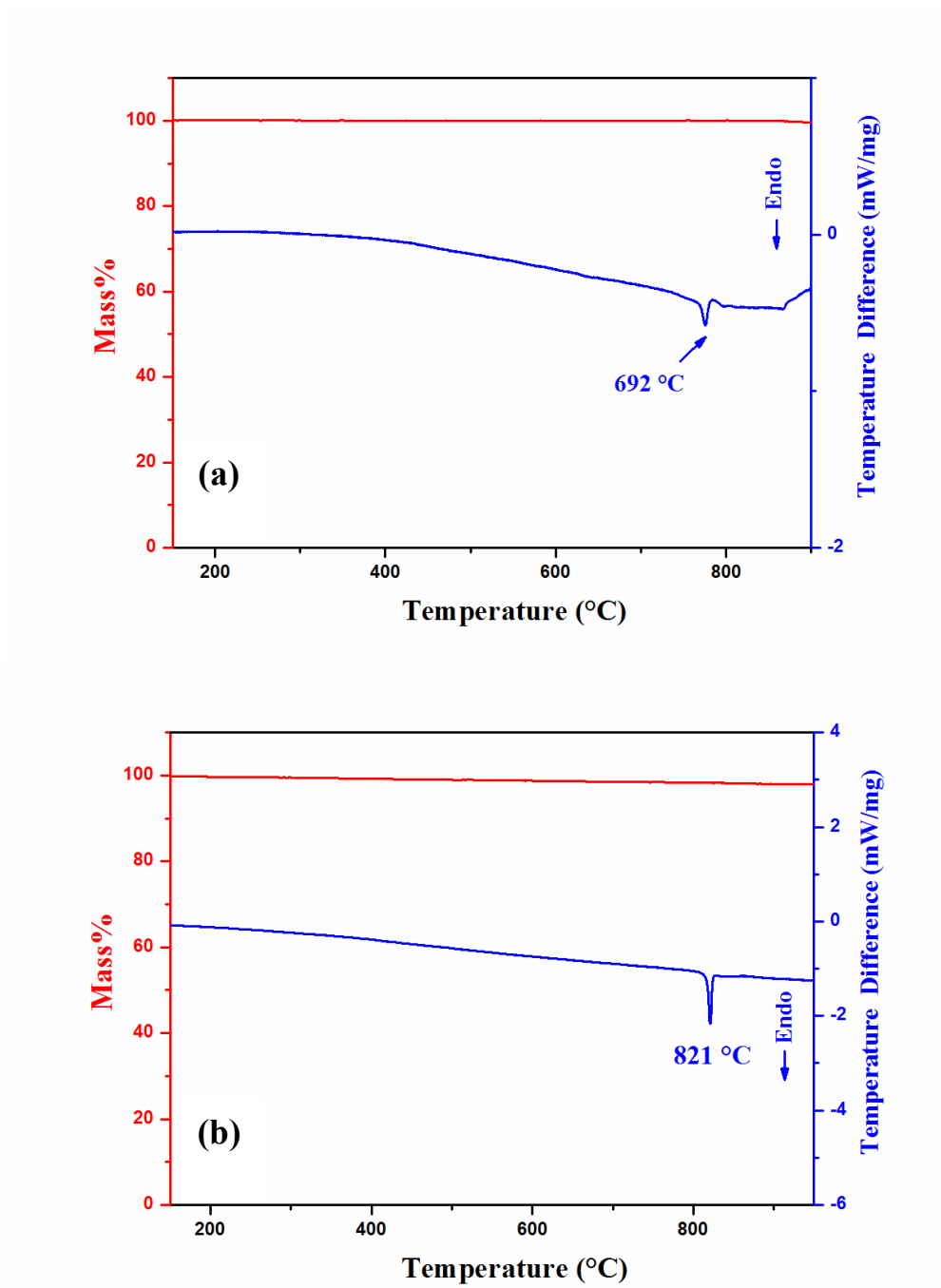

Fig. S3 TGA/DSC curves of (a) $Pb_4O(BO_3)(PO_4)$ and (b) $Bi_4O_3(BO_3)(PO_4)$.

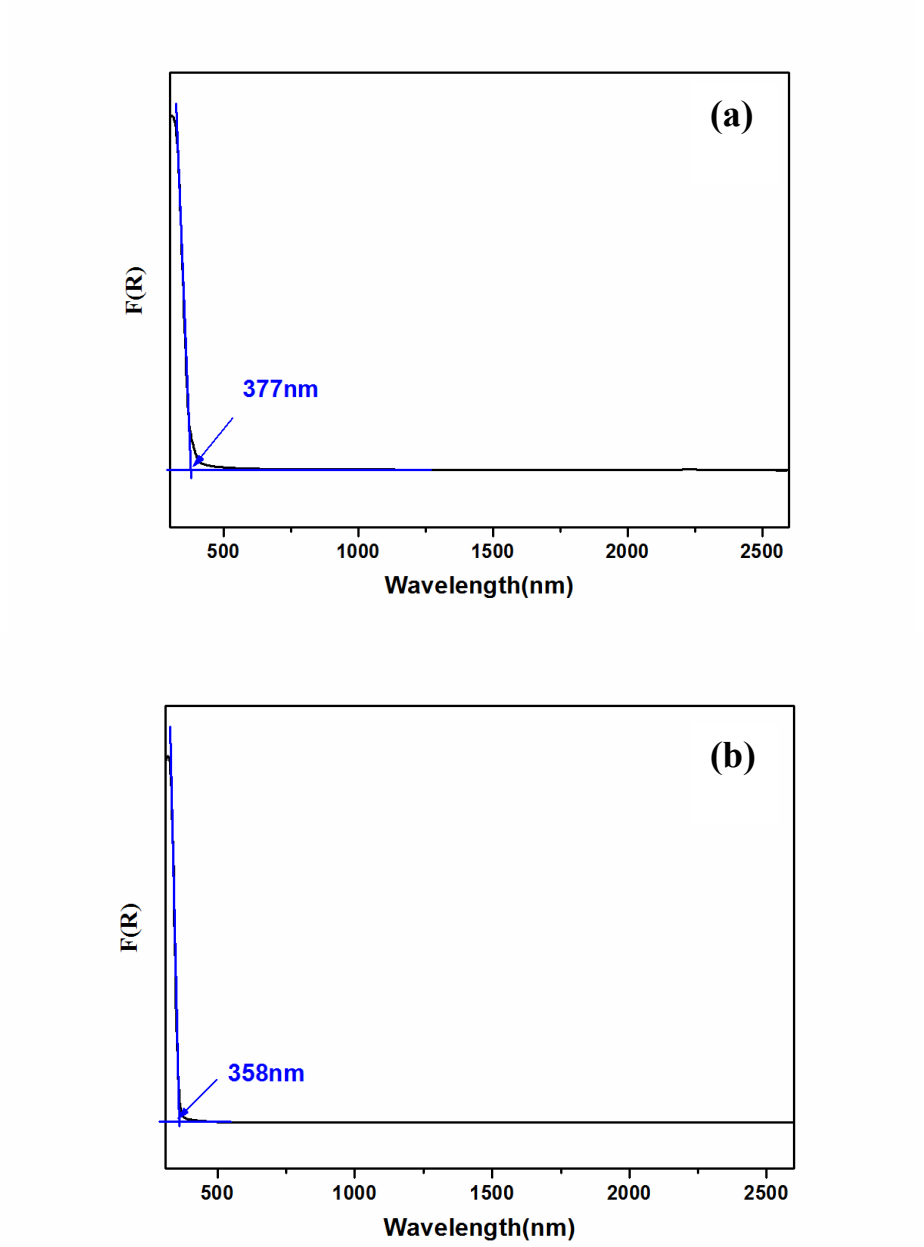

Fig. S4 UV-vis–NIR diffuse reflectance spectroscopy of (a) $Pb_4O(BO_3)(PO_4)$ and (b) $Bi_4O_3(BO_3)(PO_4)$.