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Supporting Information

Application of the dimensional reduction formalism to $Pb_{9-x}Ba_x[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (x = 0, 2, 6, 7): a series of phosphates with two types of isolated polyphosphate groups

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Table S1 Phosphates with two types of isolated P-O groups

$[P_2O_7]\&[P_3O_{10}]$	$AM_6(P_2O_7)_2(P_3O_{10})$ (A = Ag, K, Na, M = Mn; A = K, M = Cd, Mg)	
	$CsMo_4O_4(P_2O_7)_2(P_3O_{10})$	$Cs_2Mo_5O_2(P_2O_7)_2(P_3O_{10})$
	$Na_7Y_2(P_2O_7)_2(P_3O_{10})$	
$[PO_4]\&[P_3O_{10}]$	$U_2(PO_4)(P_3O_{10})$	$CsTa_2(PO_4)_2(P_3O_{10})$
$[PO_4]\&[P_2O_7]$	$Th_4(PO_4)_4(P_2O_7)$	$BaMo_2O_3(PO_4)(P_2O_7)$
	$Cs_xMo_6O_2(PO_4)_2(P_2O_7)_4$ (x = 3, 4)	$Pb_2Mo_2O(PO_4)_2(P_2O_7)$
	$Na_4Ni_5(PO_4)_2(P_2O_7)_2$	$Rb_6Bi_4(PO_4)_2(P_2O_7)_3$
	$AM_2(PO_4)(P_2O_7)$ (A = Ag, M = V, Cr; A = Mo, M = Pb; A = Mn, M= Sr; A = Si, M = Eu; A = V, M = Ca)	
	$AM_3(PO_4)(P_2O_7)$ (A= Li, M = Mg; A = K, M = Ni; A = Th, M = Na)	
	$Li_9M_3(PO_4)_2(P_2O_7)_3$ (M = Al, Ga, Cr, Fe, V, Mo)	
	$Na_7M_4(PO_4)(P_2O_7)_4$ (M = V, Fe, Al, Cr, In)	
	$Na_4M_3(PO_4)_2(P_2O_7)$ (M = Mn, Co, Ni, Mg, Fe)	
	$AMo_2O_2(PO_4)(P_2O_7)$ (M = Ag, K, Rb, Cs, Tl)	
	$M_3Ti_3O(PO_4)_3(P_2O_7)$ (M = K, Rb, Tl)	
	$Ni_4M_2(PO_4)_2(P_2O_7)$ (M = K, Tl)	

Table S2 Atomic coordinates (× 10^4)，equivalent isotropic displacement parameters ($Å^2$× 10^3) and BVS for $Pb_{9-x}Ba_x[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (x = 0, 2, 6, 7).

Atom	x	y	z	Wyck.	U_{eq}[a]	BVS[b,c]
			$Pb_9[Li_2(P_2O_7)_2(P_4O_{13})_2]$			
Li(1)	10000(30)	5060(40)	6919(19)	2i	18(6)	1.00
Pb(1)	10000	0	10000	1a	20(1)	1.82
Pb(2)	2358(1)	6408(1)	4947(1)	2i	12(1)	1.87
Pb(3)	6064(1)	6971(1)	9953(1)	2i	11(1)	1.95
Pb(4)	4103(1)	6751(1)	7508(1)	2i	19(1)	1.60
Pb(5)	8343(1)	10010(1)	7518(1)	2i	24(1)	1.48
P(1)	10313(4)	5976(4)	8778(2)	2i	5(1)	4.81
P(2)	7862(5)	3639(5)	8528(2)	2i	8(1)	5.01
P(3)	3315(5)	10354(4)	8409(2)	2i	6(1)	5.00
P(4)	3893(5)	12597(4)	6739(2)	2i	6(1)	5.02
P(5)	1824(5)	10448(4)	5889(2)	2i	6(1)	4.98
P(6)	2750(5)	12631(5)	4244(2)	2i	6(1)	4.96
O(1)	10394(14)	6516(13)	7792(7)	2i	13(2)	1.85
O(2)	8958(13)	7366(13)	9217(7)	2i	10(2)	1.94
O(3)	12223(13)	5549(14)	9137(7)	2i	12(2)	1.85
O(4)	9531(13)	4137(12)	8988(6)	2i	8(2)	2.08
O(5)	7655(15)	1792(13)	8994(8)	2i	17(2)	1.85
O(6)	6182(14)	5019(14)	8716(8)	2i	18(2)	1.93
O(7)	3225(14)	12027(13)	3374(7)	2i	12(2)	1.86
O(8)	917(13)	13901(13)	4280(6)	2i	8(2)	1.91
O(9)	4245(14)	13361(14)	4582(7)	2i	14(2)	1.83
O(10)	2474(14)	10796(12)	4895(6)	2i	9(2)	2.08
O(11)	19(13)	11600(15)	6072(7)	2i	15(2)	1.87
O(12)	1924(15)	8495(13)	6150(7)	2i	14(2)	1.85
O(13)	3397(13)	10937(13)	6391(7)	2i	10(2)	2.18
O(14)	2608(14)	14285(13)	6443(7)	2i	12(2)	1.93
O(15)	3505(14)	12195(13)	7769(7)	2i	12(2)	2.05
O(16)	5880(14)	12525(14)	6560(7)	2i	15(2)	1.89
O(17)	1672(16)	9699(16)	8180(8)	2i	23(3)	1.79
O(18)	5093(15)	9055(14)	8269(8)	2i	18(2)	1.87
O(19)	3080(15)	10864(14)	9312(8)	2i	17(2)	2.11
O(20)	8431(17)	3610(16)	7592(7)	2i	21(2)	1.89
			$Pb_7Ba_2[Li_2(P_2O_7)_2(P_4O_{13})_2]$			
Li(1)	60(30)	4910(40)	3091(18)	2i	18(6)	0.97
Pb(1)	0	0	0	1a	25(1)	1.78
Pb(2)	3926(1)	3023(1)	41(1)	2i	13(1)	1.90
Pb(3)	2348(1)	6417(1)	4945(1)	2i	18(1)	1.77
Pb(4)	5899(1)	3280(1)	2498(1)	2i	26(1)	1.46
Ba(5)	1653(1)	36(1)	2468(1)	2i	6(1)	2.14

P(1)	-312(5)	4049(5)	1224(2)	2i	8(1)	4.92
P(2)	2159(5)	6349(5)	1460(2)	2i	10(1)	4.89
P(3)	2744(5)	2617(5)	4241(2)	2i	8(1)	4.91
P(4)	1822(5)	468(5)	5896(2)	2i	9(1)	4.97
P(5)	3877(5)	2590(5)	6741(2)	2i	9(1)	4.98
P(6)	3314(5)	346(5)	8413(2)	2i	8(1)	5.03
O(1)	-2203(14)	4483(14)	867(7)	2i	13(2)	1.86
O(2)	1028(15)	2645(14)	789(7)	2i	13(2)	1.94
O(3)	-418(14)	3527(14)	2196(7)	2i	11(2)	1.97
O(4)	468(14)	5860(14)	1006(7)	2i	12(2)	2.06
O(5)	2326(16)	8204(15)	1008(8)	2i	20(2)	1.90
O(6)	3831(16)	4985(16)	1254(9)	2i	24(3)	1.90
O(7)	1660(20)	6300(20)	2414(8)	2i	32(3)	1.85
O(8)	3187(17)	2007(15)	3373(7)	2i	18(2)	1.94
O(9)	931(14)	3901(14)	4287(7)	2i	14(2)	1.90
O(10)	4257(14)	3349(15)	4571(8)	2i	18(2)	1.73
O(11)	2466(15)	820(14)	4897(7)	2i	12(2)	2.07
O(12)	47(15)	1651(18)	6076(8)	2i	23(3)	1.93
O(13)	1877(17)	-1458(14)	6153(7)	2i	19(2)	1.81
O(14)	3397(15)	935(15)	6392(7)	2i	16(2)	2.18
O(15)	2597(14)	4275(14)	6453(7)	2i	13(2)	1.88
O(16)	5858(16)	2515(16)	6555(7)	2i	18(2)	1.94
O(17)	3498(17)	2172(14)	7768(7)	2i	16(2)	2.03
O(18)	1729(18)	-352(17)	8173(9)	2i	27(3)	1.89
O(19)	5087(16)	-924(15)	8277(8)	2i	18(2)	1.96
O(20)	3041(17)	863(15)	9312(7)	2i	19(2)	2.08
			$Pb_3Ba_6[Li_2(P_2O_7)_2(P_4O_{13})_2]$			
Li(1)	50(30)	4940(30)	3092(13)	2i	21(5)	0.93
Pb(1)	10000	10000	0	1a	36(1)	1.64
Pb(2)	6085(1)	6986(1)	-39(1)	2i	18(1)	1.93
Ba(1)	5895(1)	3336(1)	2514(1)	2i	11(1)	1.91
Ba(2)	2361(1)	6456(1)	4935(1)	2i	7(1)	2.45
Ba(3)	1636(1)	69(1)	2451(1)	2i	12(1)	2.06
P(1)	10304(4)	5916(4)	-1227(2)	2i	11(1)	4.91
P(2)	7270(4)	7415(4)	5755(2)	2i	11(1)	4.91
P(3)	8176(4)	9513(4)	4084(2)	2i	11(1)	5.00
P(4)	6145(4)	7422(4)	3240(2)	2i	12(1)	4.94
P(5)	6674(4)	9674(4)	1584(2)	2i	12(1)	4.97
P(6)	7805(4)	3661(4)	-1450(2)	2i	14(1)	5.02
O(1)	9489(12)	4116(11)	-1011(5)	2i	16(2)	2.04
O(2)	9057(12)	6134(12)	5715(6)	2i	17(2)	2.09
O(3)	7544(12)	9214(11)	5074(5)	2i	14(2)	2.01
O(4)	8969(12)	7324(12)	-798(6)	2i	16(2)	1.94
O(5)	6564(14)	7830(12)	2220(6)	2i	21(2)	2.03

O(6)	4890(13)	10911(12)	1713(6)	2i	21(2)	2.04
O(7)	9932(12)	8325(13)	3896(6)	2i	21(2)	2.06
O(8)	8120(14)	11441(12)	3818(6)	2i	21(2)	1.97
O(9)	6842(14)	8061(12)	6610(5)	2i	20(2)	2.03
O(10)	4165(13)	7479(13)	3420(6)	2i	22(2)	1.98
O(11)	6608(12)	9052(11)	3603(6)	2i	16(2)	2.15
O(12)	12160(13)	5470(12)	-865(6)	2i	19(2)	1.92
O(13)	10410(13)	6439(12)	-2196(5)	2i	17(2)	2.03
O(14)	7683(14)	1803(12)	-1029(6)	2i	23(2)	1.94
O(15)	6138(13)	4964(14)	-1186(7)	2i	28(2)	2.02
O(16)	5748(13)	6698(12)	5450(6)	2i	22(2)	1.86
O(17)	7410(13)	5732(12)	3532(6)	2i	19(2)	2.02
O(18)	8217(16)	3794(16)	-2401(6)	2i	32(3)	1.83
O(19)	6945(14)	9143(13)	691(6)	2i	24(2)	2.05
O(20)	8278(14)	10359(14)	1813(7)	2i	27(2)	1.86
			$Pb_2Ba_7[Li_2(P_2O_7)_2(P_4O_{13})_2]$			
Li(1)	110(20)	4900(20)	3089(11)	2i	21(3)	0.90
Ba(1)	10000	10000	0	1a	17(1)	2.31
Pb(2)	6071(1)	6999(1)	-40(1)	2i	20(1)	1.85
Ba(3)	5899(1)	3382(1)	2529(1)	2i	12(1)	1.79
Ba(4)	2379(1)	6486(1)	4931(1)	2i	9(1)	2.30
Ba(5)	1626(1)	85(1)	2449(1)	2i	11(1)	2.03
P(1)	10291(3)	5900(3)	-1232(1)	2i	9(1)	4.86
P(2)	7270(3)	7429(3)	5751(1)	2i	9(1)	4.88
P(3)	8176(3)	9504(3)	4074(1)	2i	9(1)	5.03
P(4)	6155(3)	7421(3)	3236(1)	2i	9(1)	4.97
P(5)	6665(3)	9684(3)	1586(1)	2i	10(1)	4.99
P(6)	7765(3)	3678(3)	-1455(2)	2i	11(1)	4.98
O(1)	9481(8)	4095(8)	-1020(4)	2i	13(1)	1.94
O(2)	9052(8)	6138(8)	5709(4)	2i	14(1)	2.02
O(3)	7555(8)	9208(8)	5058(4)	2i	14(1)	2.00
O(4)	8985(8)	7307(8)	-811(4)	2i	15(1)	2.00
O(5)	6571(9)	7835(8)	2219(4)	2i	16(1)	2.01
O(6)	4890(9)	10912(9)	1731(5)	2i	19(1)	2.00
O(7)	9913(9)	8332(9)	3884(4)	2i	18(1)	2.06
O(8)	8122(9)	11430(8)	3808(4)	2i	17(1)	1.95
O(9)	6842(9)	8116(9)	6592(4)	2i	17(1)	1.97
O(10)	4187(8)	7471(9)	3414(5)	2i	19(1)	1.97
O(11)	6608(8)	9042(8)	3600(4)	2i	13(1)	2.17
O(12)	12152(8)	5426(9)	-867(4)	2i	17(1)	1.87
O(13)	10410(8)	6436(8)	-2199(4)	2i	13(1)	2.01
O(14)	7673(9)	1792(9)	-1053(5)	2i	20(1)	2.05
O(15)	6105(9)	4946(9)	-1163(5)	2i	22(2)	1.99
O(16)	5750(8)	6711(8)	5459(4)	2i	17(1)	1.86

O(17)	7389(9)	5722(8)	3526(4)	2i	16(1)	1.99
O(18)	8122(11)	3890(11)	-2400(5)	2i	30(2)	1.83
O(19)	6905(10)	9175(9)	695(4)	2i	23(2)	2.15
O(20)	8264(9)	10360(9)	1809(5)	2i	21(1)	1.90

[a]U(eq) is defined as the one-third of the trace of the orthogonalized U_{ij} tensor;

[b]Band valences calculated with the program Band Valences Calculator Version 2.00, C. Hormillosa, S. Healy, T. Stephen, McMaster University, 1993;

[c]Valence sums calculated with the formula: $S_i = \exp[(R_0-R_i)/B]$, where S_i = valence of band "i" and B = 0.37.

Table S3 Selected bond distances (Å) for $Pb_{9-x}Ba_x[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (x = 0, 2, 6, 7).

$Pb_9[Li_2(P_2O_7)_2(P_4O_{13})_2]$			
Li(1)-O(1)	1.97(3)	Pb(5)-O(16)	2.737(11)
Li(1)-O(20)	1.90(3)	Pb(5)-O(7)#6	2.732(10)
Li(1)-O(14)#3	2.03(3)	P(1)-O(1)	1.522(11)
Li(1)-O(8)#6	2.02(3)	P(1)-O(2)	1.535(10)
Pb(1)-O(5)#1	2.493(11)	P(1)-O(4)	1.613(10)
Pb(1)-O(5)	2.493(11)	P(2)-O(20)	1.485(11)
Pb(1)-O(19)#2	2.598(11)	P(2)-O(5)	1.523(11)
Pb(1)-O(19)#3	2.598(11)	P(2)-O(6)	1.523(11)
Pb(2)-O(11)#4	2.573(11)	P(2)-O(4)	1.616(10)
Pb(2)-O(14)#5	2.617(10)	P(3)-O(17)	1.495(13)
Pb(2)-O(12)	2.633(10)	P(3)-O(19)	1.509(12)
Pb(2)-O(9)#5	2.631(11)	P(3)-O(18)	1.523(11)
Pb(2)-O(8)#4	2.654(9)	P(3)-O(15)	1.621(11)
Pb(2)-O(16)#6	2.677(11)	P(4)-O(16)	1.469(11)
Pb(2)-O(9)#6	2.727(10)	P(4)-O(14)	1.494(10)
Pb(3)-O(2)	2.396(10)	P(4)-O(15)	1.595(11)
Pb(3)-O(19)#8	2.386(11)	P(4)-O(13)	1.590(10)
Pb(3)-O(3)#9	2.423(10)	P(5)-O(12)	1.490(10)
Pb(3)-O(6)	2.625(12)	P(5)-O(11)	1.496(10)
Pb(4)-O(18)	2.545(12)	P(5)-O(10)	1.577(10)
Pb(4)-O(6)	2.564(11)	P(5)-O(13)	1.591(10)
Pb(4)-O(7)#6	2.558(10)	P(6)-O(7)	1.498(11)
Pb(5)-O(11)#10	2.708(11)	P(6)-O(9)	1.503(11)
Pb(5)-O(17)#10	2.707(12)	P(6)-O(8)	1.523(10)
P(1)-O(3)	1.523(10)	P(6)-O(10)	1.641(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+2; #2 -x+1,-y+1,-z+2; #3 x+1,y-1,z; #4 -x,-y+2,-z+1; #5 x,y-1,z; #6 -x+1,-y+2,-z+1; #7 x-1,y,z; #8 -x+1,-y+2,-z+2; #9 -x+2,-y+1,-z+2; #10 x+1,y,z; #11 x-1,y+1,z; #12 x,y+1,z

$Pb_7Ba_2[Li_2(P_2O_7)_2(P_4O_{13})_2]$			
Li(1)-O(3)	2.00(3)	Ba(5)-O(7)#2	2.931(14)
Li(1)-O(7)	1.90(3)	Ba(5)-O(2)	3.049(11)
Li(1)-O(9)	2.01(3)	Ba(5)-P(2)#2	3.450(4)
Li(1)-O(15)#1	2.07(3)	Ba(5)-P(4)#5	3.519(4)
Pb(1)-O(5)#2	2.497(12)	Ba(5)-P(5)#9	3.749(4)
Pb(1)-O(5)#3	2.497(12)	P(1)-O(3)	1.505(11)
Pb(1)-O(20)#4	2.588(12)	P(1)-O(2)	1.543(11)
Pb(1)-O(20)#5	2.588(12)	P(1)-O(1)	1.515(10)
Pb(2)-O(20)#4	2.401(12)	P(1)-O(4)	1.604(11)
Pb(2)-O(2)	2.417(10)	P(2)-O(7)	1.503(13)
Pb(2)-O(1)#3	2.423(11)	P(2)-O(6)	1.528(12)
Pb(2)-O(6)	2.617(13)	P(2)-O(5)	1.524(12)

Pb(3)-O(12)#1	2.577(11)	P(2)-O(4)	1.632(11)
Pb(3)-O(9)#1	2.672(11)	P(3)-O(8)	1.504(11)
Pb(3)-O(15)	2.649(10)	P(3)-O(10)	1.519(11)
Pb(3)-O(10)	2.670(12)	P(3)-O(9)	1.525(11)
Pb(3)-O(13)#7	2.675(11)	P(3)-O(11)	1.629(11)
Pb(3)-O(16)#8	2.691(11)	P(4)-O(12)	1.497(12)
Pb(3)-O(10)#8	2.747(10)	P(4)-O(13)	1.482(11)
Pb(4)-O(19)#9	2.606(12)	P(4)-O(11)	1.591(11)
Pb(4)-O(6)	2.602(12)	P(4)-O(14)	1.588(11)
Pb(4)-O(8)	2.610(12)	P(5)-O(15)	1.495(11)
Ba(5)-O(8)	2.709(12)	P(5)-O(16)	1.474(12)
Ba(5)-O(18)#5	2.742(13)	P(5)-O(14)	1.593(11)
Ba(5)-O(16)#9	2.787(12)	P(5)-O(17)	1.597(11)
Ba(5)-O(12)#5	2.772(12)	P(6)-O(18)	1.490(12)
Ba(5)-O(5)#2	2.852(13)	P(6)-O(19)	1.516(12)
Ba(5)-O(19)#9	2.768(12)	P(6)-O(20)	1.514(11)
Ba(5)-O(3)	2.846(10)	P(6)-O(17)	1.623(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1; #2 x,y-1,z; #3 -x,-y+1,-z; #4 x,y,z-1; #5 -x,-y,-z+1; #6 -x,-y,-z; #7 x,y+1,z; #8 -x+1,-y+1,-z+1; #9 -x+1,-y,-z+1; #10 x,y,z+1

$Pb_3Ba_6[Li_2(P_2O_7)_2(P_4O_{13})_2]$

Li(1)-O(18)#1	1.94(2)	Ba(3)-O(7)#11	2.792(9)
Li(1)-O(13)#1	2.01(2)	Ba(3)-O(14)#12	2.826(10)
Li(1)-O(17)#2	2.05(2)	Ba(3)-O(13)#1	2.839(9)
Li(1)-O(2)#3	2.04(2)	Ba(3)-O(10)#9	2.831(9)
Pb(1)-O(14)#5	2.535(10)	Ba(3)-O(18)#12	3.016(11)
Pb(1)-O(14)#6	2.535(10)	Ba(3)-O(4)#1	3.033(9)
Pb(1)-O(19)#7	2.614(10)	P(1)-O(13)	1.509(9)
Pb(1)-O(19)	2.614(10)	P(1)-O(12)	1.511(9)
Pb(2)-O(19)	2.410(10)	P(1)-O(4)	1.537(9)
Pb(2)-O(12)#6	2.424(9)	P(1)-O(1)	1.620(9)
Pb(2)-O(4)	2.419(9)	P(2)-O(2)	1.511(9)
Pb(2)-O(15)	2.584(10)	P(2)-O(9)	1.501(9)
Ba(1)-O(9)#3	2.685(9)	P(2)-O(16)	1.519(9)
Ba(1)-O(6)#9	2.703(10)	P(2)-O(3)	1.655(9)
Ba(1)-O(15)#1	2.706(11)	P(3)-O(8)	1.490(9)
Ba(1)-O(8)#9	2.798(10)	P(3)-O(7)	1.493(9)
Ba(1)-O(13)#6	2.816(9)	P(3)-O(11)	1.589(9)
Ba(1)-O(20)#9	2.946(11)	P(3)-O(3)	1.578(8)
Ba(1)-O(12)#6	2.963(9)	P(4)-O(10)	1.485(10)
Ba(1)-O(17)	3.095(9)	P(4)-O(17)	1.497(9)
Ba(2)-O(7)#2	2.614(9)	P(4)-O(11)	1.592(9)
Ba(2)-O(17)#3	2.712(9)	P(4)-O(5)	1.597(9)
Ba(2)-O(10)	2.712(10)	P(5)-O(19)	1.515(9)

Ba(2)-O(16)#3	2.724(10)	P(5)-O(20)	1.511(10)
Ba(2)-O(8)#10	2.720(9)	P(5)-O(6)	1.509(9)
Ba(2)-O(2)#2	2.709(9)	P(5)-O(5)	1.624(9)
Ba(2)-O(16)	2.797(9)	P(6)-O(18)	1.491(10)
Ba(2)-O(2)#3	2.838(9)	P(6)-O(14)	1.510(9)
Ba(3)-O(9)#3	2.710(9)	P(6)-O(15)	1.523(10)
Ba(3)-O(20)#11	2.759(10)	P(6)-O(1)	1.624(9)
Ba(3)-O(6)#9	2.766(9)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z; #2 x-1,y,z; #3 -x+1,-y+1,-z+1; #4 -x,-y+1,-z+1; #5 x,y+1,z; #6 -x+2,-y+1,-z; #7 -x+2,-y+2,-z; #8 x+1,y+1,z; #9 x,y-1,z; #10 -x+1,-y+2,-z+1; #11 x-1,y-1,z; #12 -x+1,-y,-z; #13 x+1,y,z

$Pb_2Ba_7[Li_2(P_2O_7)_2(P_4O_{13})_2]$

Li(1)-O(18)#1	1.937(19)	Ba(4)-O(2)#2	2.865(6)
Li(1)-O(13)#1	1.999(18)	Ba(5)-O(9)#2	2.707(7)
Li(1)-O(2)#2	2.042(17)	Ba(5)-O(6)#8	2.767(6)
Li(1)-O(17)#3	2.119(18)	Ba(5)-O(20)#10	2.774(7)
Ba(1)-O(14)#5	2.570(7)	Ba(5)-O(7)#10	2.799(7)
Ba(1)-O(14)#6	2.570(7)	Ba(5)-O(14)#11	2.811(7)
Ba(1)-O(19)	2.641(7)	Ba(5)-O(13)#1	2.835(6)
Ba(1)-O(19)#7	2.641(7)	Ba(5)-O(10)#8	2.860(7)
Ba(1)-O(4)#7	2.903(6)	Ba(5)-O(4)#1	3.027(7)
Ba(1)-O(4)	2.903(6)	Ba(5)-O(18)#11	3.098(8)
Ba(1)-O(20)	3.072(7)	P(1)-O(13)	1.517(6)
Ba(1)-O(20)#7	3.072(7)	P(1)-O(12)	1.522(7)
Ba(1)-O(1)#5	3.306(6)	P(1)-O(4)	1.527(6)
Ba(1)-O(1)#6	3.306(6)	P(1)-O(1)	1.622(6)
Pb(2)-O(19)	2.427(7)	P(2)-O(9)	1.504(7)
Pb(2)-O(12)#6	2.427(7)	P(2)-O(2)	1.518(6)
Pb(2)-O(4)	2.451(6)	P(2)-O(16)	1.512(6)
Pb(2)-O(15)	2.588(7)	P(2)-O(3)	1.659(6)
Ba(3)-O(9)#2	2.735(6)	P(3)-O(7)	1.482(7)
Ba(3)-O(6)#8	2.741(7)	P(3)-O(8)	1.491(6)
Ba(3)-O(15)#1	2.745(7)	P(3)-O(3)	1.578(7)
Ba(3)-O(8)#8	2.795(7)	P(3)-O(11)	1.587(6)
Ba(3)-O(13)#6	2.814(6)	P(4)-O(10)	1.481(6)
Ba(3)-O(20)#8	2.992(7)	P(4)-O(17)	1.494(7)
Ba(3)-O(12)#6	2.993(7)	P(4)-O(11)	1.587(6)
Ba(3)-O(17)	3.040(6)	P(4)-O(5)	1.601(7)
Ba(3)-O(16)#2	3.306(7)	P(5)-O(20)	1.503(7)
Ba(4)-O(7)#3	2.644(7)	P(5)-O(6)	1.510(7)
Ba(4)-O(10)	2.723(7)	P(5)-O(19)	1.515(7)
Ba(4)-O(2)#3	2.736(6)	P(5)-O(5)	1.627(7)
Ba(4)-O(8)#9	2.742(7)	P(6)-O(18)	1.483(7)
Ba(4)-O(17)#2	2.743(6)	P(6)-O(14)	1.519(7)

Ba(4)-O(16)#2	2.759(6)	P(6)-O(15)	1.525(7)
Ba(4)-O(16)	2.797(6)	P(6)-O(1)	1.633(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z; #2 -x+1,-y+1,-z+1; #3 x-1,y,z; #4 -x,-y+1,-z+1; #5 x,y+1,z; #6 -x+2,-y+1,-z; #7 -x+2,-y+2,-z; #8 x,y-1,z; #9 -x+1,-y+2,-z+1; #10 x-1,y-1,z; #11 -x+1,-y,-z; #12 x+1,y+1,z; #13 x+1,y,z

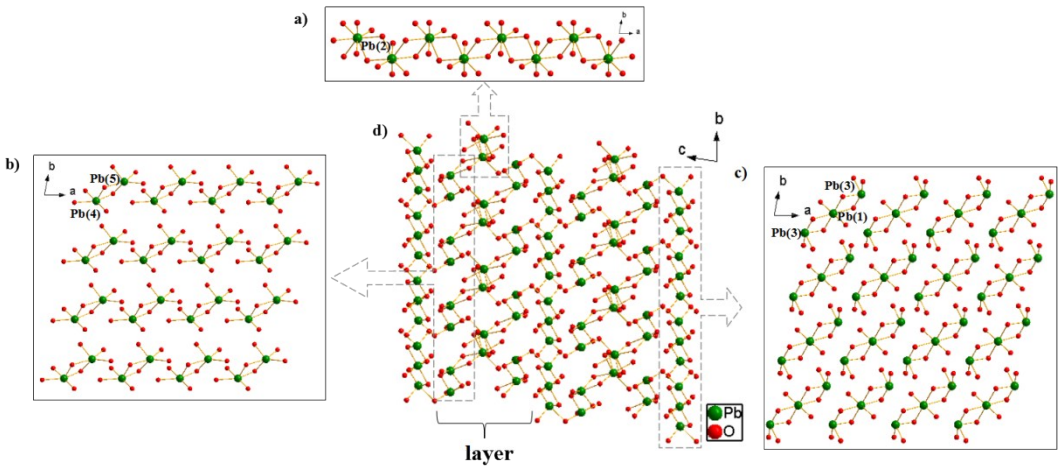

Figure S1. Ball−stick representation of the PbO_6 chain (a), the Pb_2O_8 dimer (b), the Pb_3O_{10} trimer (c) and the 3D Pb-O framework (d).

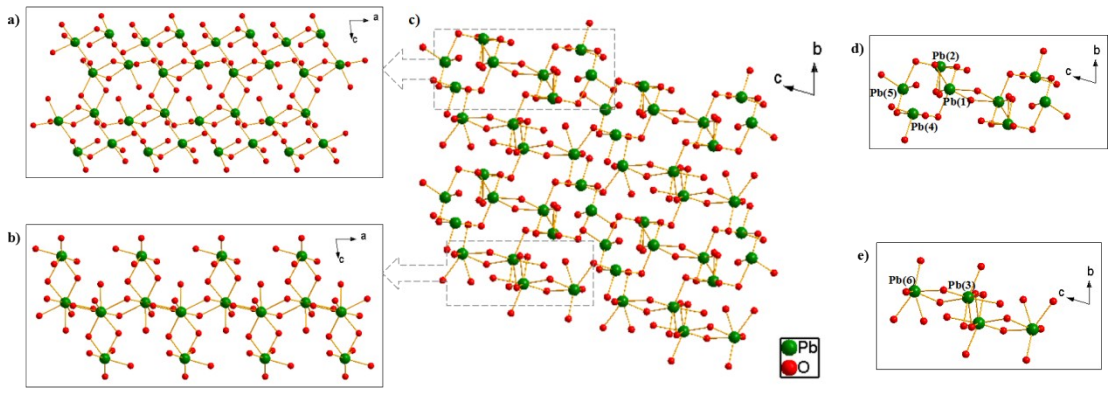

Figure S2. Ball−stick representation of the 1D ribbon (a), the chain (b), the 3D Pb-O framework (c), the $(Pb_4O_{14})O_2(Pb_4O_{14})$ unit (d) and the $(Pb_2O_{10})O_2(Pb_2O_{10})$ unit (e).

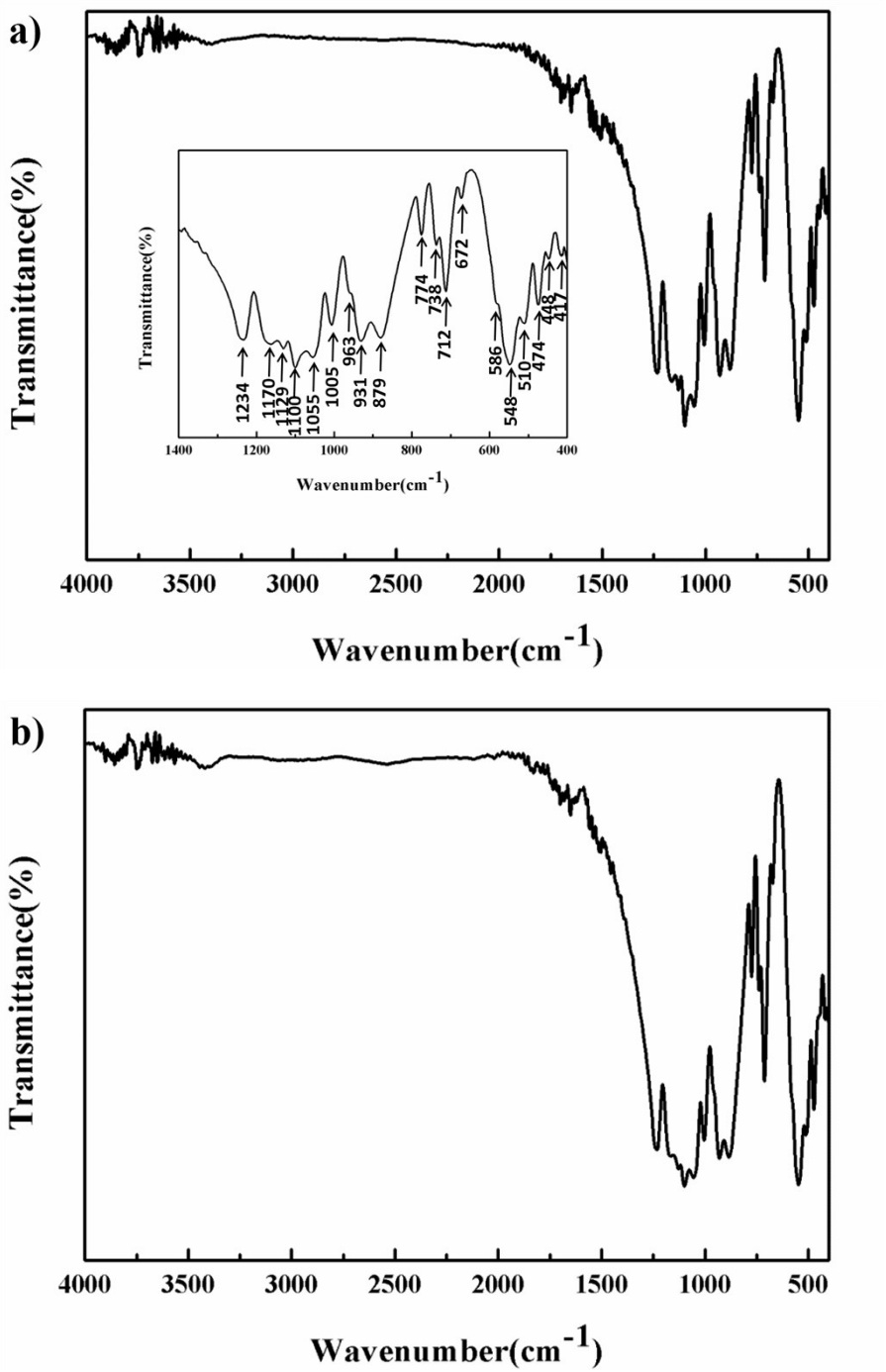

Figure S3. IR Spectroscopy of $Pb_2Ba_7[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (a) and $Pb_3Ba_6[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (b).

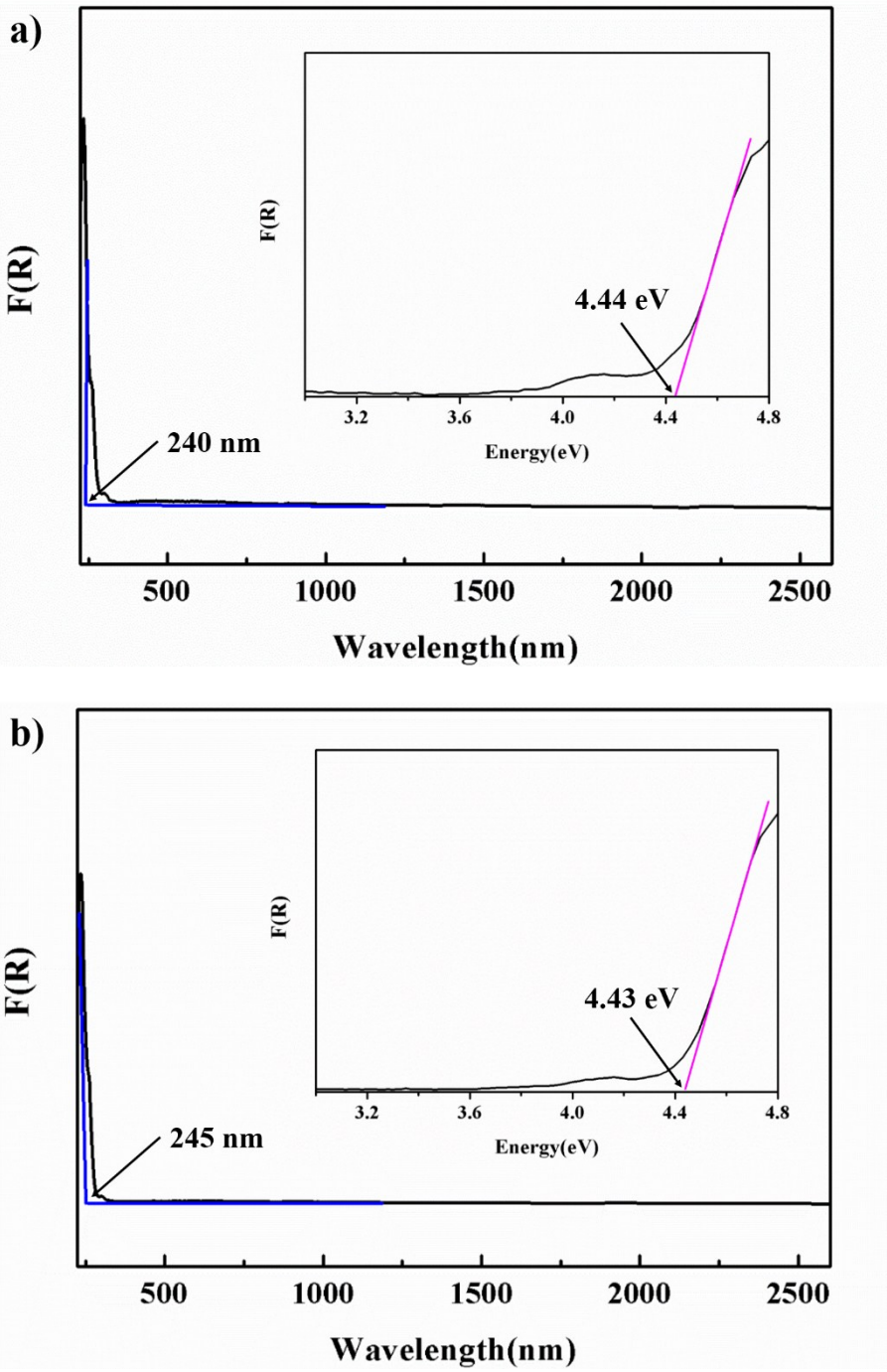

Figure S4. UV-Vis-NIR diffuse-reflectance spectroscopy of $Pb_2Ba_7[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (a) and $Pb_3Ba_6[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (b).

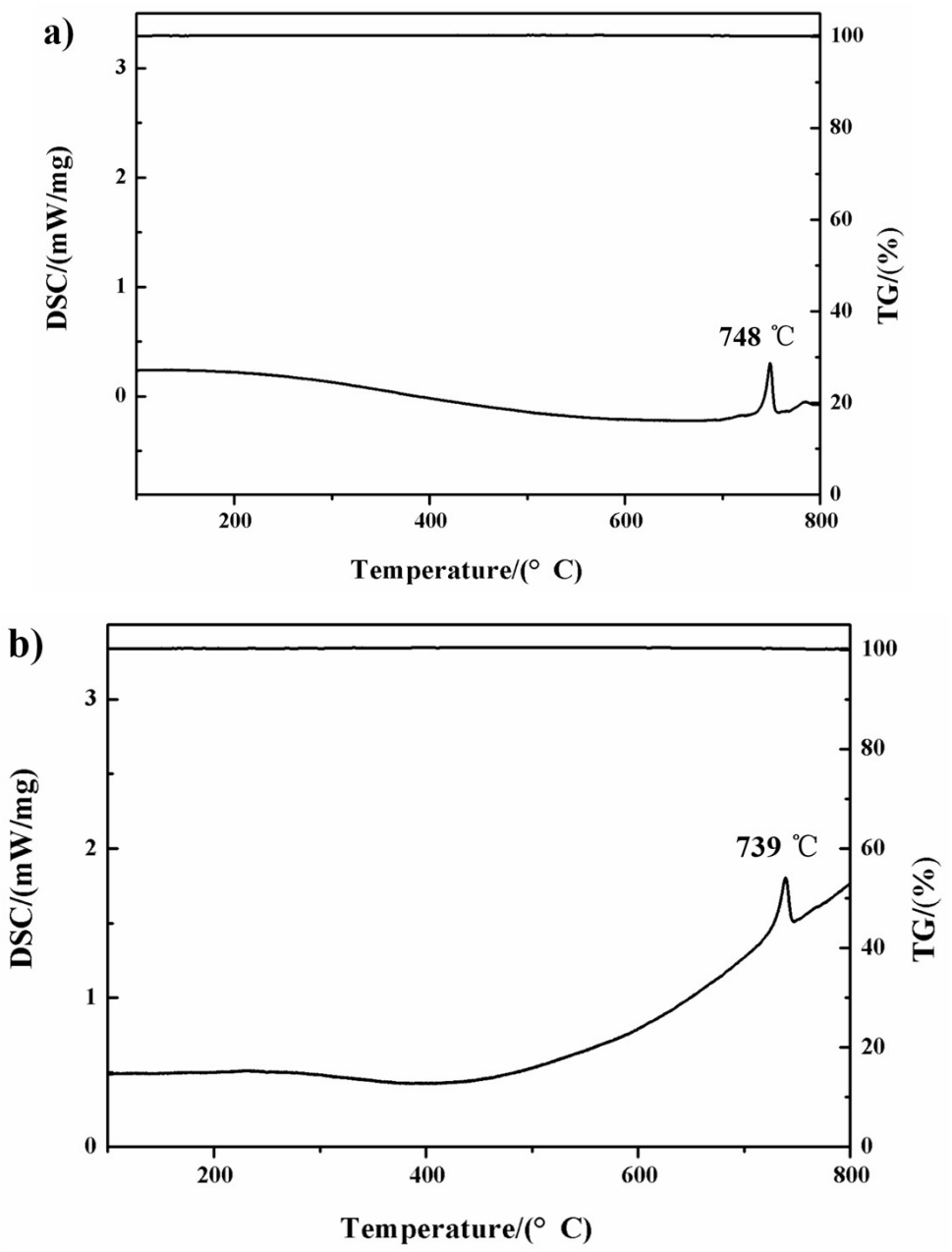

Figure S5. TGA and DSC curves of $Pb_2Ba_7[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (a) and $Pb_3Ba_6[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (b).

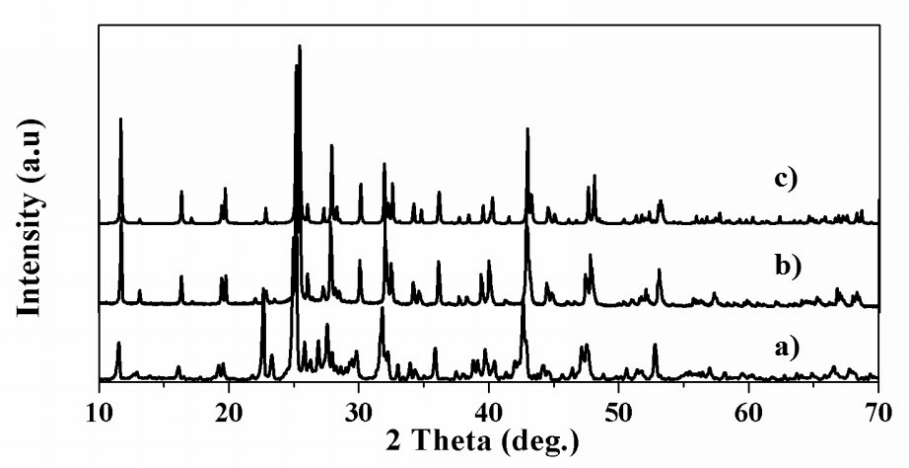

Figure S6. X-ray diffraction patterns of solidified melt of $Pb_2Ba_7[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (a) and $Pb_3Ba_6[Li_2(P_2O_7)_2(P_4O_{13})_2]$ (b) and the X-ray diffraction patterns of $PbBaP_2O_7$ (PDF-#83-0888) (c).

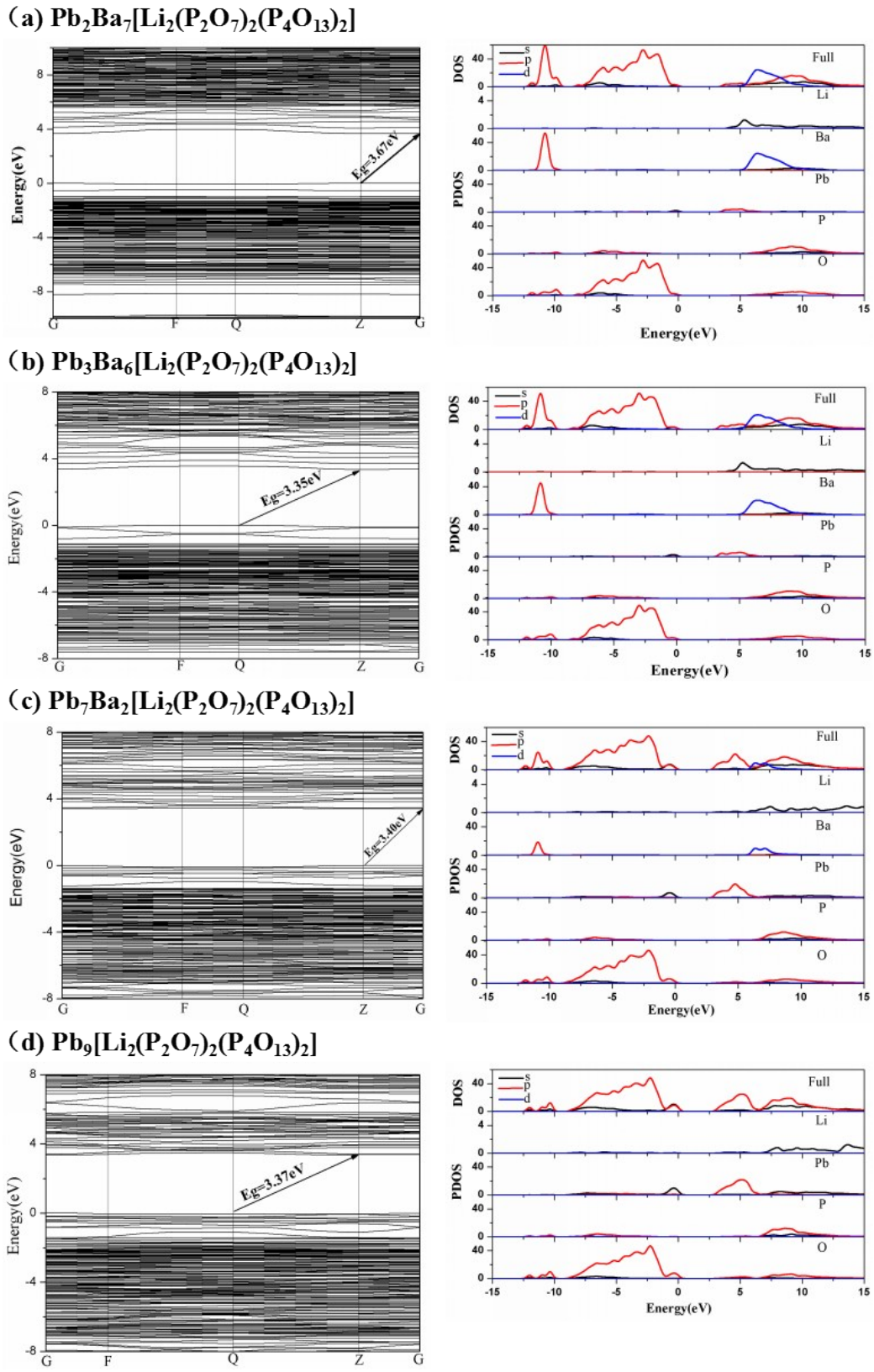

Figure S7. The band structures (left) and projected density of states (PDOS) (right) of the crystals.