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An alkali metal phosphate $RbPbBi_2(PO_4)_3$ with three kinds of disorder: The effect of isolated soft cation units on the crystal structure

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Table S1. Crystal data and structure refinements for $RbPbBi_2(PO_4)_3$.

Empirical formula	$RbPbBi_2(PO_4)_3$
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	$P3_121$
Formula weight	995.53
a (Å)	7.191(6)
b (Å)	7.191(6)
c (Å)	6.563(11)
Z, Volume (Å^3)	1, 293.9(7)
ρ_{Calcd} (Mg/m^3)	5.624
μ(/mm)	48.724
F(000)	426
R(int)	0.0589
Goodness-of-fit on F^2	1.075
Final R indices [$F_o^2>2\sigma(F_o^2)$][a]	R1 = 0.0355, wR2 = 0.0789
R indices (all data)[a]	R1 = 0.0503, wR2 = 0.0880
Absolute structure parameter	0.05(4)
Largest diff. peak and hole (e·Å^{-3})	3.715 and -2.455

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w F_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $RbPbBi_2(PO_4)_3$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Bi(1)	0	4961(2)	11667	16(1)
Pb(1)	0	4961(2)	11667	16(1)
Rb(11)	470(20)	280(30)	9445(18)	3(3)
Rb(12)	400(30)	0	8333	3(3)
P(1)	0	4469(12)	6667	10(2)
O(1)	1200(30)	6330(30)	8210(20)	23(5)
O(2)	-1490(20)	2480(30)	7940(30)	19(4)

Table S3. Selected bond distances (Å) and angles (deg) for $RbPbBi_2(PO_4)_3$.

Bi(1)-O(2)#1	2.282(15)	O(2)#1-Bi(1)-O(1)#4	78.6(5)
Bi(1)-O(2)#2	2.282(15)	O(2)#2-Bi(1)-O(1)#4	162.2(5)
Bi(1)-O(1)	2.454(18)	O(1)-Bi(1)-O(1)#4	80.1(6)
Bi(1)-O(1)#3	2.454(18)	O(1)#3-Bi(1)-O(1)#4	114.0(5)
Bi(1)-O(1)#4	2.67(2)	O(2)#1-Bi(1)-O(1)#5	162.2(5)
Bi(1)-O(1)#5	2.67(2)	O(2)#2-Bi(1)-O(1)#5	78.6(5)
Rb(11)-O(2)	2.78(2)	O(1)-Bi(1)-O(1)#5	114.0(5)
Rb(11)-O(2)#8	2.83(2)	O(1)#3-Bi(1)-O(1)#5	80.1(6)
Rb(11)-O(2)#7	2.92(2)	O(1)#4-Bi(1)-O(1)#5	117.5(7)
Rb(11)-O(1)#10	2.94(2)	O(2)-Rb(11)-O(2)#8	67.9(7)
Rb(11)-O(2)#6	2.96(2)	O(2)-Rb(11)-O(2)#7	164.4(5)
Rb(11)-O(1)#10	3.24(2)	O(2)#8-Rb(11)-O(2)#7	115.1(6)
Rb(11)-O(1)#10	3.24(2)	O(2)-Rb(11)-O(1)#10	95.2(6)
Rb(12)-O(2)#8	2.74(3)	O(2)#8-Rb(11)-O(1)#10	155.9(7)
Rb(12)-O(2)	2.74(3)	O(2)#7-Rb(11)-O(1)#10	85.9(6)
Rb(12)-O(1)#11	2.97(3)	O(2)-Rb(11)-O(2)#6	115.3(5)
Rb(12)-O(1)#10	2.97(3)	O(2)#8-Rb(11)-O(2)#6	51.0(6)
Rb(12)-O(2)#8	3.202(3)	O(2)#7-Rb(11)-O(2)#6	64.4(7)
Rb(12)-O(2)	3.202(3)	O(1)#10-Rb(11)-O(2)#6	149.4(8)
Rb(12)-O(2)#8	3.312(3)	O(2)#8-Rb(12)-O(2)	69.6(8)
Rb(12)-O(2)	3.312(3)	O(2)#8-Rb(12)-O(1)#11	95.4(5)
P(1)-O(2)	1.536(16)	O(2)-Rb(12)-O(1)#11	162.6(7)
P(1)-O(2)#12	1.536(16)	O(2)#8-Rb(12)-O(1)#10	162.6(7)
P(1)-O(1)#12	1.551(18)	O(2)-Rb(12)-O(1)#10	95.4(5)
P(1)-O(1)	1.551(18)	O(1)#11-Rb(12)-O(1)#10	100.7(9)
O(2)#1-Bi(1)-O(2)#2	86.7(8)	O(2)-P(1)-O(2)#12	108.8(14)
O(2)#1-Bi(1)-O(1)	74.6(6)	O(2)-P(1)-O(1)#12	113.8(8)
O(2)#2-Bi(1)-O(1)	86.3(6)	O(2)#12-P(1)-O(1)#12	106.2(10)
O(2)#1-Bi(1)-O(1)#3	86.3(6)	O(2)-P(1)-O(1)	106.2(10)
O(2)#2-Bi(1)-O(1)#3	74.6(6)	O(2)#12-P(1)-O(1)	113.8(8)
O(1)-Bi(1)-O(1)#3	153.8(8)	O(1)#12-P(1)-O(1)	108.3(13)

#1 y,x+1,-z+2 #2 -y,x-y+1,z+1/3 #3 -x,-x+y,-z+7/3
#4 -y+1,x-y+1,z+1/3 #5 y-1,x,-z+2
#6 -y,x-y,z+1/3 #7 y,x,-z+2 #8 x-y,-y,-z+5/3
#9 -x+y,-x,z-1/3 #10 x-y+1,-y+1,-z+5/3
#11 x,y-1,z #12 -x,-x+y,-z+4/3 #13 x-y,-y+1,-z+5/3
#14 -x+y,-x+1,z-1/3 #15 x,y+1,z #16 -x+y-1,-x,z-1/3

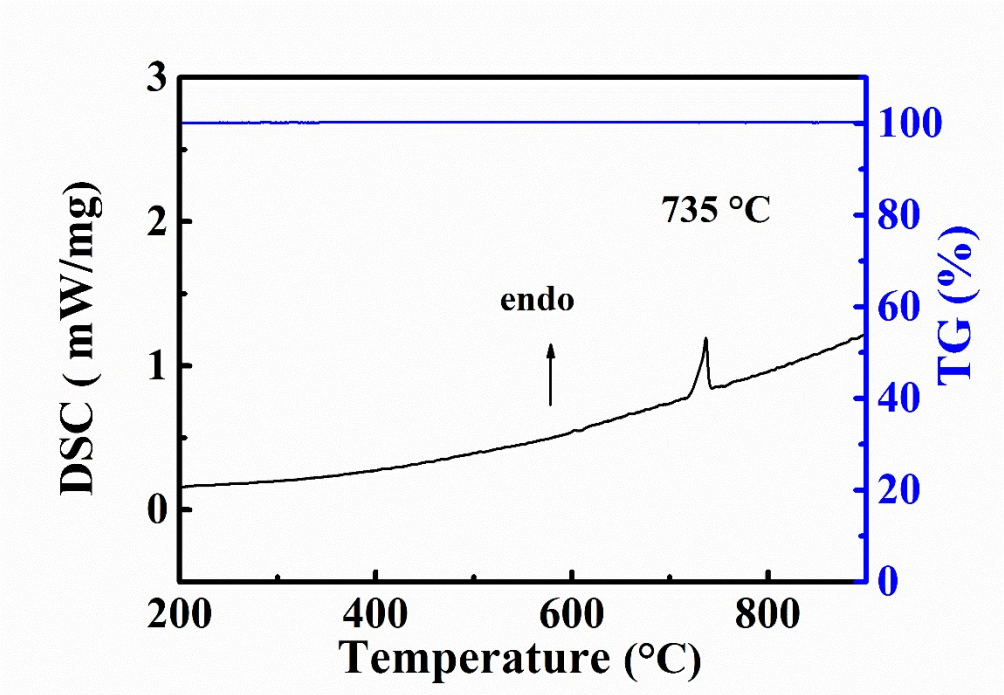

Fig. S1. TG-DSC curves of $RbPbBi_2(PO_4)_3$.

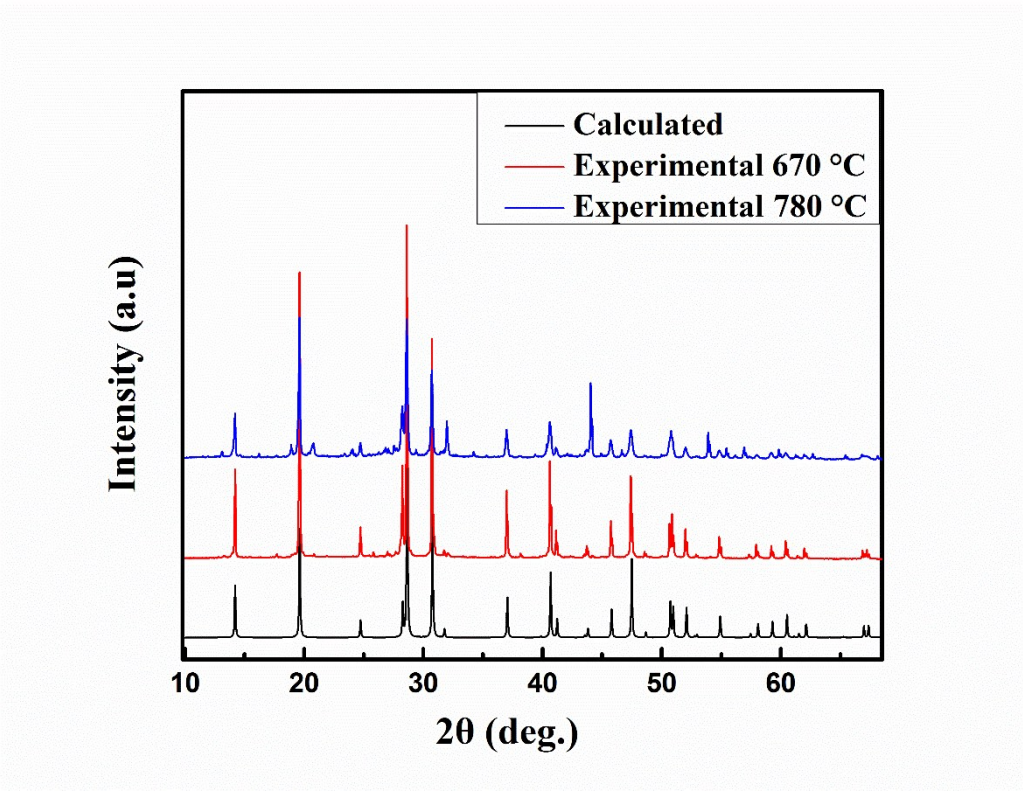

Fig. S2. Experimental and calculated XRD patterns of $RbPbBi_2(PO_4)_3$.

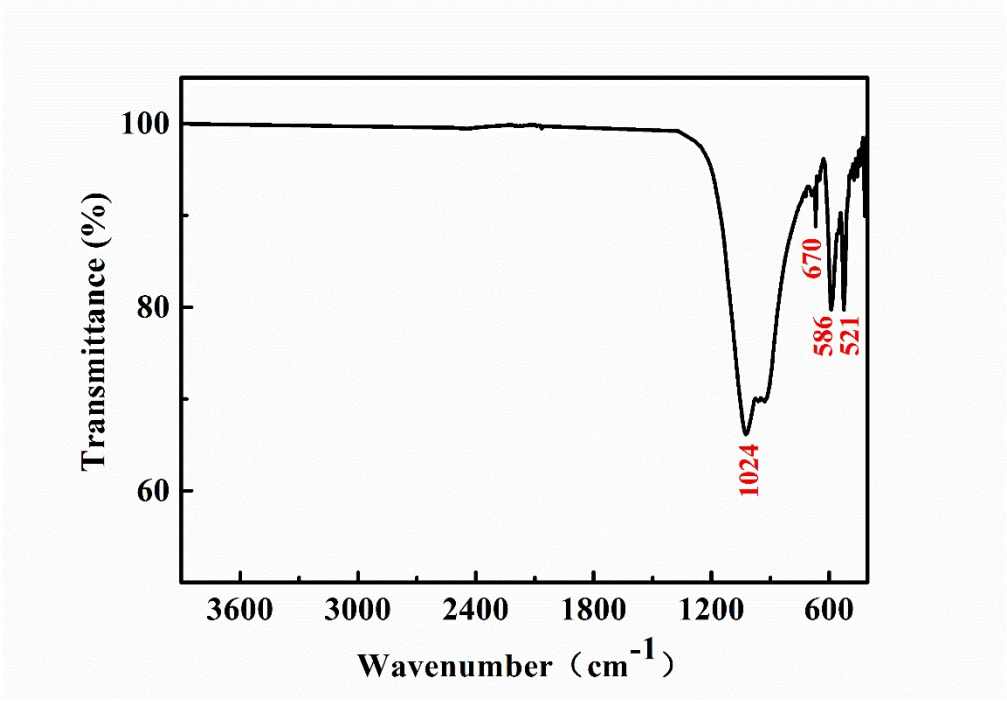

Fig. S3. IR spectrum of $RbPbBi_2(PO_4)_3$.