Electronic Supplementary Information

Three non-centrosymmetric bismuth phosphates, Li$_2$ABi(PO$_4$)$_2$ (A = K, Rb, and Cs): effects of cation on the crystal structure and SHG response

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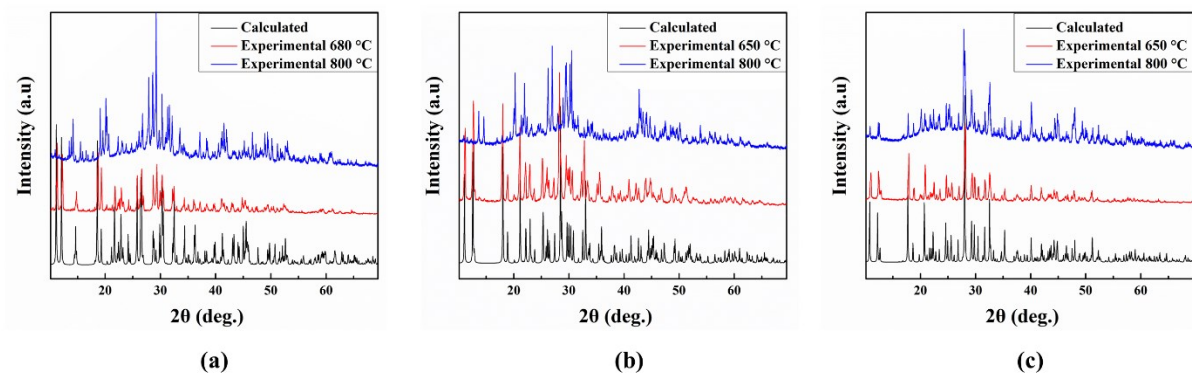
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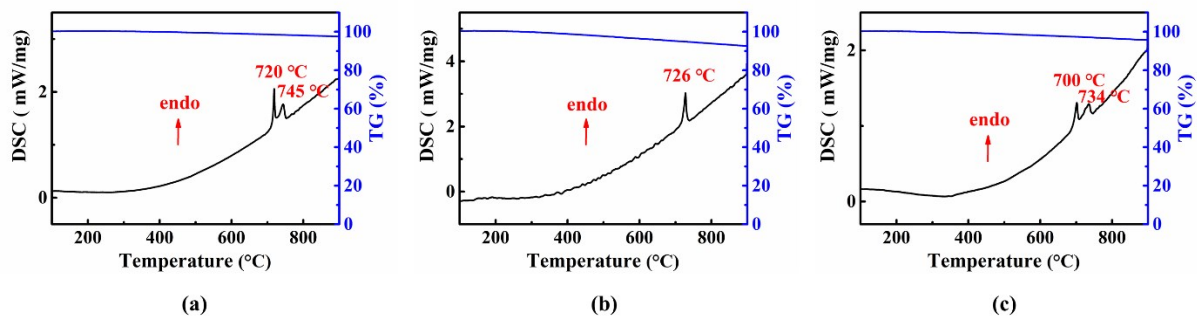
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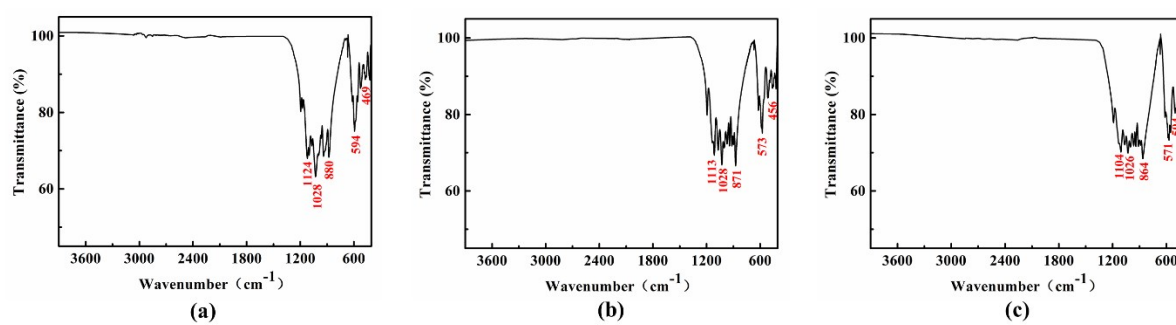
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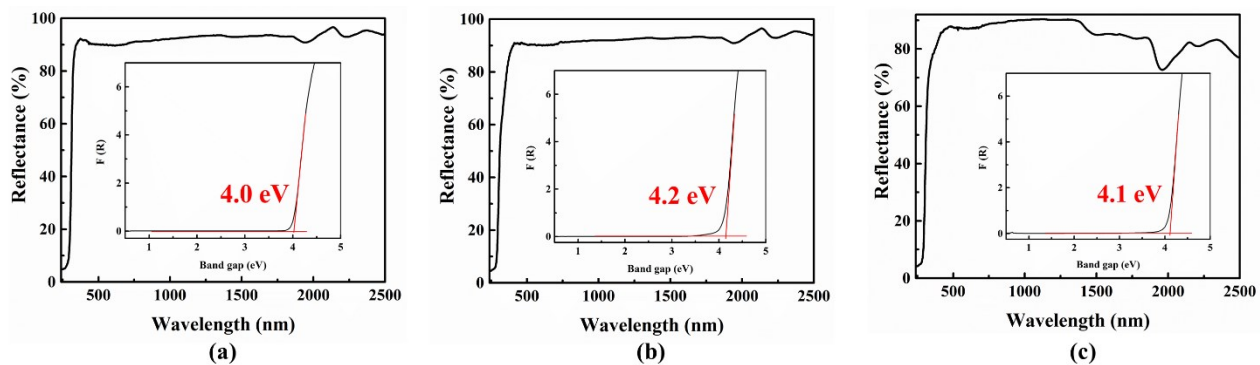
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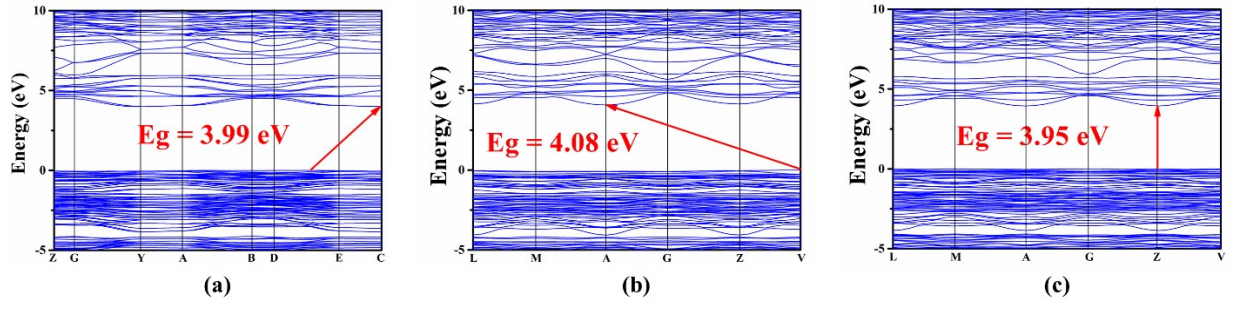
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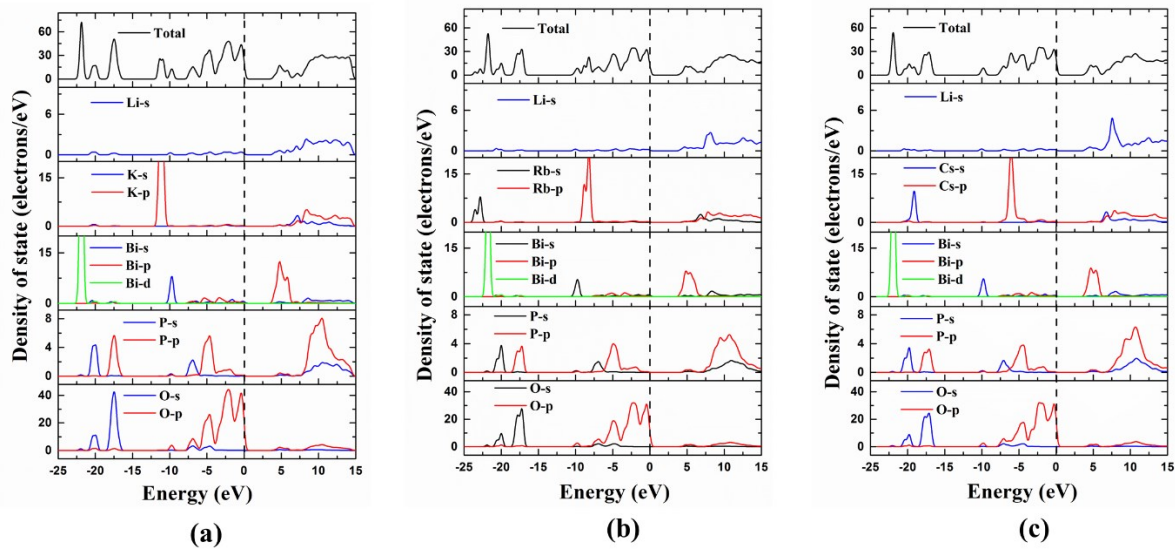
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Table S1. Crystal data and structure refinements for $Li_2KBi(PO_4)_2$, $Li_2RbBi(PO_4)_2$, and $Li_2CsBi(PO_4)_2$.

Empirical formula	$Li_2KBi(PO_4)_2$	$Li_2RbBi(PO_4)_2$	$Li_2CsBi(PO_4)_2$
Temperature		296(2) K	
Wavelength		0.71073 Å	
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1$	$C2$	$C2$
Formula weight	451.90	498.27	545.71
a (Å)	7.940(6)	28.17(5)	28.56(4)
b (Å)	4.948(3), β=90.67º	4.994(9), β= 91.34º	5.084(7), β= 92.32º
c (Å)	18.403	7.996(14)	8.211(11)
Z, Volume (Å³)	4, 723.0(9)	6, 1124(3)	6, 1192(3)
ρ_{Calcd} (Mg/m³)	4.152	4.415	4.563
μ(/mm)	25.413	30.409	27.124
F(000)	808	1320	1428
R(int)	0.0679	0.1158	0.0654
Goodness-of-fit on F^2	0.944	0.952	0.913
Final R indices $[F_o^2>2\sigma(F_o^2)]^a$	$R_1 = 0.0587$, $wR_2 = 0.1027$	$R_1 = 0.0637$ $wR_2 = 0.1072$	$R_1 = 0.0597$ $wR_2 = 0.0985$
R indices (all data)[a]	$R_1 = 0.0745$, $wR_2 = 0.1116$	$R_1 = 0.0866$, $wR_2 = 0.1174$	$R_1 = 0.0781$, $wR_2 = 0.1064$
Largest diff. peak and hole (e·Å⁻³)	2.7 and -4.9	2.3 and -2.9	2.5 and -1.9

[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 S2a. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $Li_2KBi(PO_4)_2$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Bi(1)	4953(1)	6166(2)	6100(1)	15(1)
Bi(2)	6889(1)	5952(2)	8204(1)	12(1)
K(1)	99(7)	6403(17)	6423(4)	23(2)
K(2)	3162(8)	1701(13)	9332(4)	22(2)
Li(1)	450(50)	11590(100)	8040(20)	14(10)
Li(2)	8400(50)	11350(130)	5270(20)	21(11)
Li(3)	3500(50)	11460(110)	7170(20)	16(10)
Li(4)	10310(60)	6650(100)	9110(30)	21(12)
P(1)	8054(8)	1587(16)	9330(4)	11(2)
P(2)	7244(9)	11674(16)	6901(4)	15(2)
P(3)	2775(8)	6580(15)	7910(4)	12(2)
P(4)	2441(10)	11480(20)	5485(4)	26(2)
O(1)	4370(20)	7200(40)	8404(11)	16(4)
O(2)	8030(20)	1990(40)	10153(10)	16(5)
O(3)	8850(20)	12300(40)	7324(11)	19(5)
O(4)	6900(30)	8560(40)	6867(14)	25(5)
O(5)	3150(20)	7640(40)	7136(11)	12(4)
O(6)	6410(30)	2870(40)	8979(12)	24(5)
O(7)	2500(20)	3610(40)	7893(11)	11(4)
O(8)	8040(20)	-1470(40)	9172(11)	14(5)
O(9)	7240(30)	12840(50)	6111(13)	32(6)
O(10)	5730(20)	13100(40)	7283(12)	23(5)
O(11)	9490(20)	2910(40)	8965(11)	15(4)
O(12)	1290(20)	8110(40)	8241(11)	11(4)
O(13)	2610(30)	8450(40)	5488(13)	24(5)
O(14)	3060(30)	12700(50)	6185(13)	34(6)
O(15A)	4100(50)	13040(90)	5060(20)	24(8)
O(15B)	2950(60)	12480(90)	4790(30)	24(8)
O(16A)	400(40)	11730(80)	5570(20)	21(7)
O(16B)	960(50)	12900(80)	5130(30)	21(7)

Table S2b. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$^2\times 10^3$) for Li$_2$RbBi(PO$_4$)$_2$. U$_{eq}$ is defined as one-third of the trace of the orthogonalized U$_{ij}$ tensor.

Atom	x	y	z	U(eq)
Bi(1)	6322(1)	10665(3)	1896(1)	17(1)
Bi(2)	5000	885(5)	10000	17(1)
Rb(1)	7913(1)	11471(8)	1818(4)	25(1)
Rb(2)	5000	11185(14)	5000	32(2)
Li(1)	8100(20)	6200(160)	4760(70)	33(16)
Li(2)	5660(18)	6530(120)	8280(70)	19(14)
Li(3)	6186(19)	6470(130)	5560(70)	24(14)
P(1)	4529(3)	6370(20)	7797(11)	16(2)
P(2)	7047(3)	6370(20)	3156(10)	14(2)
P(3)	6127(3)	1369(19)	7794(10)	14(2)
O(1)	6104(8)	-1570(50)	7440(30)	17(6)
O(2)	4286(8)	7100(60)	6230(30)	34(7)
O(3)	5040(7)	7450(50)	7960(30)	12(5)
O(4)	6916(8)	3350(50)	3080(30)	10(5)
O(5)	4267(7)	7790(50)	9220(30)	16(6)
O(6)	7567(7)	6800(50)	3230(30)	20(6)
O(7)	6784(7)	7740(50)	4560(30)	15(5)
O(8)	6847(8)	7660(50)	1550(30)	29(7)
O(9)	6356(8)	2900(50)	6360(30)	17(6)
O(10)	6449(7)	1920(50)	9380(30)	19(5)
O(11)	4509(8)	3230(50)	8100(30)	21(6)
O(12)	5634(7)	2550(50)	8260(30)	11(5)

Table S2c. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Li_2CsBi(PO_4)_2$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Cs(1)	2871(1)	843(4)	6711(2)	20(1)
Cs(2)	5000	5736(6)	0	24(1)
Bi(1)	3691(1)	5045(2)	3087(1)	13(1)
Bi(2)	5000	5268(4)	5000	13(1)
Li(1)	3832(17)	10660(110)	-470(60)	20(12)
Li(2)	4344(18)	730(120)	6490(60)	23(13)
Li(3)	1921(17)	990(100)	330(60)	15(11)
P(1)	4523(2)	10756(16)	2850(9)	11(2)
P(2)	2978(3)	759(16)	1732(9)	11(2)
P(3)	3878(3)	5752(16)	7129(9)	14(2)
O(1)	4530(8)	7720(40)	3160(30)	17(5)
O(2)	4269(7)	12100(40)	4280(20)	14(5)
O(3)	3165(7)	2150(40)	3370(20)	9(4)
O(4)	4270(7)	11350(40)	1240(20)	17(5)
O(5)	3231(8)	2220(40)	390(30)	20(5)
O(6)	2458(7)	1070(40)	1660(30)	21(5)
O(7)	3555(7)	6020(40)	5570(20)	14(5)
O(8)	3917(8)	2880(40)	7550(30)	17(5)
O(9)	4363(7)	6890(40)	6720(20)	10(4)
O(10)	5025(7)	11830(40)	2960(20)	15(5)
O(11)	3655(7)	7300(40)	8500(20)	9(4)
O(12)	3124(8)	-2180(40)	1810(30)	16(5)

Table S3a. Selected distances (Å) and angles (deg) for Li$_2$KBi(PO$_4$)$_2$.

Bi(1)-O(14)#1	2.29(2)	O(4)#7-K(1)-O(16B)#1	130.0(10)
Bi(1)-O(4)	2.40(2)	O(9)#6-K(1)-O(16B)#1	71.6(9)
Bi(1)-O(15B)#2	2.44(5)	O(14)#1-K(1)-O(16B)#1	49.9(9)
Bi(1)-O(13)	2.44(2)	O(3)#6-K(1)-O(16B)#8	129.1(9)
Bi(1)-O(15A)#2	2.45(5)	O(16A)#1-K(1)-O(16B)#8	72.6(11)
Bi(1)-O(9)#1	2.45(2)	O(5)-K(1)-O(16B)#8	127.6(8)
Bi(1)-O(5)	2.504(19)	O(13)-K(1)-O(16B)#8	62.3(9)
Bi(1)-O(15A)#1	2.55(5)	O(4)#7-K(1)-O(16B)#8	86.6(9)
Bi(1)-O(10)#1	2.72(2)	O(9)#6-K(1)-O(16B)#8	76.1(9)
Bi(2)-O(6)	2.13(2)	O(14)#1-K(1)-O(16B)#8	102.6(9)
Bi(2)-O(1)	2.128(18)	O(16B)#1-K(1)-O(16B)#8	57.8(7)
Bi(2)-O(8)#3	2.37(2)	O(3)#6-K(1)-O(16A)	161.8(8)
Bi(2)-O(10)#1	2.38(2)	O(16A)#1-K(1)-O(16A)	114.1(14)
K(1)-O(3)#6	2.81(2)	O(5)-K(1)-O(16A)	88.9(9)
K(1)-O(16A)#1	2.81(4)	O(13)-K(1)-O(16A)	47.6(8)
K(1)-O(5)	2.81(2)	O(4)#7-K(1)-O(16A)	84.4(8)
K(1)-O(13)	2.84(2)	O(9)#6-K(1)-O(16A)	118.7(9)
K(1)-O(4)#7	2.88(2)	O(14)#1-K(1)-O(16A)	112.3(8)
K(1)-O(9)#6	2.93(2)	O(16B)#1-K(1)-O(16A)	93.8(12)
K(1)-O(14)#1	3.02(2)	O(16B)#8-K(1)-O(16A)	48.5(11)
K(1)-O(16B)#1	3.03(4)	O(3)#6-K(1)-O(15B)#8	104.6(9)
K(1)-O(16B)#8	3.05(5)	O(16A)#1-K(1)-O(15B)#8	79.8(11)
K(1)-O(16A)	3.08(4)	O(5)-K(1)-O(15B)#8	153.9(9)
K(1)-O(15B)#8	3.31(5)	O(13)-K(1)-O(15B)#8	92.8(9)
K(2)-O(2)#9	2.693(19)	O(4)#7-K(1)-O(15B)#8	59.5(9)
K(2)-O(6)	2.73(2)	O(9)#6-K(1)-O(15B)#8	53.6(9)
K(2)-O(7)	2.85(2)	O(14)#1-K(1)-O(15B)#8	124.4(9)
K(2)-O(2)#10	2.945(19)	O(16B)#1-K(1)-O(15B)#8	74.5(11)
K(2)-O(1)#1	2.974(19)	O(16B)#8-K(1)-O(15B)#8	30.9(10)
K(2)-O(11)#7	3.04(2)	O(16A)-K(1)-O(15B)#8	65.1(11)
K(2)-O(12)#1	3.05(2)	O(2)#9-K(2)-O(6)	127.2(7)
K(2)-O(8)#10	3.06(2)	O(2)#9-K(2)-O(7)	123.4(6)
K(2)-O(1)	3.36(2)	O(6)-K(2)-O(7)	82.8(7)
Li(1)-O(3)#7	1.86(5)	O(2)#9-K(2)-O(2)#10	122.7(7)
Li(1)-O(12)	1.88(5)	O(6)-K(2)-O(2)#10	101.4(6)
Li(1)-O(7)#3	1.93(5)	O(7)-K(2)-O(2)#10	87.0(6)
Li(1)-O(11)#11	1.98(5)	O(2)#9-K(2)-O(1)#1	70.8(5)
Li(2)-O(16A)#5	1.69(6)	O(6)-K(2)-O(1)#1	73.1(6)
Li(2)-O(13)#12	1.91(6)	O(7)-K(2)-O(1)#1	76.8(6)
Li(2)-O(16B)#2	1.93(7)	O(2)#10-K(2)-O(1)#1	163.4(6)
Li(2)-O(9)	1.95(5)	O(2)#9-K(2)-O(11)#7	84.7(6)
Li(2)-O(15B)#2	2.19(7)	O(6)-K(2)-O(11)#7	144.2(7)

Li(2)-O(16B)#5	2.20(6)	O(7)-K(2)-O(11)#7	64.1(5)
Li(2)-O(15A)#2	2.63(7)	O(2)#10-K(2)-O(11)#7	65.5(5)
Li(2)-P(4)#12	2.97(6)	O(1)#1-K(2)-O(11)#7	109.5(6)
Li(3)-O(7)#3	1.88(5)	O(2)#9-K(2)-O(12)#1	63.7(6)
Li(3)-O(5)	1.91(6)	O(6)-K(2)-O(12)#1	114.9(6)
Li(3)-O(14)	1.95(5)	O(7)-K(2)-O(12)#1	59.9(5)
Li(3)-O(10)	1.95(5)	O(2)#10-K(2)-O(12)#1	124.9(6)
Li(4)-O(2)#13	1.89(5)	O(1)#1-K(2)-O(12)#1	49.1(5)
Li(4)-O(12)#5	1.92(5)	O(11)#7-K(2)-O(12)#1	60.7(5)
Li(4)-O(11)	1.98(6)	O(2)#9-K(2)-O(8)#10	79.9(6)
Li(4)-O(8)#3	2.04(5)	O(6)-K(2)-O(8)#10	117.1(6)
P(1)-O(11)	1.48(2)	O(7)-K(2)-O(8)#10	132.9(6)
P(1)-O(2)	1.53(2)	O(2)#10-K(2)-O(8)#10	48.9(5)
P(1)-O(8)	1.54(2)	O(1)#1-K(2)-O(8)#10	147.6(6)
P(1)-O(6)	1.58(2)	O(11)#7-K(2)-O(8)#10	80.4(5)
P(2)-O(3)	1.52(2)	O(12)#1-K(2)-O(8)#10	127.5(5)
P(2)-O(9)	1.56(3)	O(2)#9-K(2)-O(1)	169.8(6)
P(2)-O(4)	1.56(2)	O(6)-K(2)-O(1)	55.3(6)
P(2)-O(10)	1.57(2)	O(7)-K(2)-O(1)	46.5(5)
P(3)-O(7)	1.49(2)	O(2)#10-K(2)-O(1)	62.6(5)
P(3)-O(12)	1.536(19)	O(1)#1-K(2)-O(1)	102.6(6)
P(3)-O(5)	1.55(2)	O(11)#7-K(2)-O(1)	90.4(5)
P(3)-O(1)	1.58(2)	O(12)#1-K(2)-O(1)	106.0(5)
P(4)-O(15B)	1.44(4)	O(8)#10-K(2)-O(1)	108.2(5)
P(4)-O(14)	1.50(3)	O(3)#7-Li(1)-O(12)	123(3)
P(4)-O(13)	1.51(2)	O(3)#7-Li(1)-O(7)#3	112(2)
P(4)-O(16B)	1.51(4)	O(12)-Li(1)-O(7)#3	102(2)
P(4)-O(16A)	1.63(4)	O(3)#7-Li(1)-O(11)#11	106(2)
P(4)-O(15A)	1.73(4)	O(12)-Li(1)-O(11)#11	106(2)
O(14)#1-Bi(1)-O(4)	138.7(8)	O(7)#3-Li(1)-O(11)#11	107(2)
O(14)#1-Bi(1)-O(15B)#2	134.6(11)	O(16A)#5-Li(2)-O(13)#12	124(3)
O(4)-Bi(1)-O(15B)#2	79.6(12)	O(16A)#5-Li(2)-O(16B)#2	88(3)
O(14)#1-Bi(1)-O(13)	83.1(8)	O(13)#12-Li(2)-O(16B)#2	108(3)
O(4)-Bi(1)-O(13)	121.8(7)	O(16A)#5-Li(2)-O(9)	99(3)
O(15B)#2-Bi(1)-O(13)	95.2(13)	O(13)#12-Li(2)-O(9)	100(3)
O(14)#1-Bi(1)-O(15A)#2	123.5(12)	O(16B)#2-Li(2)-O(9)	140(3)
O(4)-Bi(1)-O(15A)#2	97.0(11)	O(16A)#5-Li(2)-O(15B)#2	125(4)
O(15B)#2-Bi(1)-O(15A)#2	25.4(14)	O(13)#12-Li(2)-O(15B)#2	104(3)
O(13)-Bi(1)-O(15A)#2	70.3(12)	O(16B)#2-Li(2)-O(15B)#2	49(2)
O(14)#1-Bi(1)-O(9)#1	89.0(8)	O(9)-Li(2)-O(15B)#2	98(2)
O(4)-Bi(1)-O(9)#1	81.6(7)	O(16A)#5-Li(2)-O(16B)#5	29.2(19)
O(15B)#2-Bi(1)-O(9)#1	70.9(13)	O(13)#12-Li(2)-O(16B)#5	96(3)
O(13)-Bi(1)-O(9)#1	151.1(8)	O(16B)#2-Li(2)-O(16B)#5	91(2)
O(15A)#2-Bi(1)-O(9)#1	91.6(11)	O(9)-Li(2)-O(16B)#5	114(3)

O(14)#1-Bi(1)-O(5)	77.6(7)	O(15B)#2-Li(2)-O(16B)#5	139(3)
O(4)-Bi(1)-O(5)	77.2(7)	O(16A)#5-Li(2)-O(15A)#2	148(4)
O(15B)#2-Bi(1)-O(5)	146.4(11)	O(13)#12-Li(2)-O(15A)#2	82(2)
O(13)-Bi(1)-O(5)	77.2(7)	O(16B)#2-Li(2)-O(15A)#2	64(2)
O(15A)#2-Bi(1)-O(5)	137.3(11)	O(9)-Li(2)-O(15A)#2	93(2)
O(9)#1-Bi(1)-O(5)	128.2(7)	O(15B)#2-Li(2)-O(15A)#2	23.5(17)
O(14)#1-Bi(1)-O(15A)#1	55.1(10)	O(16B)#5-Li(2)-O(15A)#2	152(3)
O(4)-Bi(1)-O(15A)#1	155.1(11)	O(7)#3-Li(3)-O(5)	121(2)
O(15B)#2-Bi(1)-O(15A)#1	80.5(14)	O(7)#3-Li(3)-O(14)	114(3)
O(13)-Bi(1)-O(15A)#1	74.9(11)	O(5)-Li(3)-O(14)	105(2)
O(15A)#2-Bi(1)-O(15A)#1	69.9(8)	O(7)#3-Li(3)-O(10)	95(2)
O(9)#1-Bi(1)-O(15A)#1	77.8(11)	O(5)-Li(3)-O(10)	123(3)
O(5)-Bi(1)-O(15A)#1	127.0(10)	O(14)-Li(3)-O(10)	97(2)
O(14)#1-Bi(1)-O(10)#1	70.7(8)	O(2)#13-Li(4)-O(12)#5	106(2)
O(4)-Bi(1)-O(10)#1	70.5(7)	O(2)#13-Li(4)-O(11)	114(3)
O(15B)#2-Bi(1)-O(10)#1	122.4(13)	O(12)#5-Li(4)-O(11)	112(3)
O(13)-Bi(1)-O(10)#1	142.4(7)	O(2)#13-Li(4)-O(8)#3	122(3)
O(15A)#2-Bi(1)-O(10)#1	147.0(11)	O(12)#5-Li(4)-O(8)#3	104(2)
O(9)#1-Bi(1)-O(10)#1	57.1(7)	O(11)-Li(4)-O(8)#3	98(2)
O(5)-Bi(1)-O(10)#1	71.2(6)	O(11)-P(1)-O(2)	114.1(11)
O(15A)#1-Bi(1)-O(10)#1	108.7(10)	O(11)-P(1)-O(8)	110.6(11)
O(6)-Bi(2)-O(1)	85.2(7)	O(2)-P(1)-O(8)	108.4(12)
O(6)-Bi(2)-O(8)#3	87.2(8)	O(11)-P(1)-O(6)	105.8(12)
O(1)-Bi(2)-O(8)#3	93.9(7)	O(2)-P(1)-O(6)	109.5(11)
O(6)-Bi(2)-O(10)#1	89.0(8)	O(8)-P(1)-O(6)	108.2(12)
O(1)-Bi(2)-O(10)#1	86.4(7)	O(3)-P(2)-O(9)	113.3(12)
O(8)#3-Bi(2)-O(10)#1	176.1(8)	O(3)-P(2)-O(4)	111.5(12)
O(3)#6-K(1)-O(16A)#1	76.7(9)	O(9)-P(2)-O(4)	109.1(14)
O(3)#6-K(1)-O(5)	101.0(6)	O(3)-P(2)-O(10)	108.8(12)
O(16A)#1-K(1)-O(5)	111.2(9)	O(9)-P(2)-O(10)	104.9(13)
O(3)#6-K(1)-O(13)	150.7(7)	O(4)-P(2)-O(10)	109.1(13)
O(16A)#1-K(1)-O(13)	83.6(9)	O(7)-P(3)-O(12)	112.5(11)
O(5)-K(1)-O(13)	66.2(6)	O(7)-P(3)-O(5)	110.3(12)
O(3)#6-K(1)-O(4)#7	77.4(6)	O(12)-P(3)-O(5)	110.9(11)
O(16A)#1-K(1)-O(4)#7	123.1(9)	O(7)-P(3)-O(1)	108.7(11)
O(5)-K(1)-O(4)#7	123.0(7)	O(12)-P(3)-O(1)	106.9(11)
O(13)-K(1)-O(4)#7	131.9(7)	O(5)-P(3)-O(1)	107.4(10)
O(3)#6-K(1)-O(9)#6	53.2(6)	O(15B)-P(4)-O(14)	122(2)
O(16A)#1-K(1)-O(9)#6	57.7(9)	O(15B)-P(4)-O(13)	109(2)
O(5)-K(1)-O(9)#6	152.3(7)	O(14)-P(4)-O(13)	111.6(15)
O(13)-K(1)-O(9)#6	130.3(7)	O(15B)-P(4)-O(16B)	71(2)
O(4)#7-K(1)-O(9)#6	66.1(6)	O(14)-P(4)-O(16B)	115.6(19)
O(3)#6-K(1)-O(14)#1	86.0(6)	O(13)-P(4)-O(16B)	122(2)
O(16A)#1-K(1)-O(14)#1	49.2(9)	O(15B)-P(4)-O(16A)	110(2)

O(5)-K(1)-O(14)#1	62.0(6)	O(14)-P(4)-O(16A)	101.9(18)
O(13)-K(1)-O(14)#1	64.7(6)	O(13)-P(4)-O(16A)	99.3(17)
O(4)#7-K(1)-O(14)#1	163.2(7)	O(16B)-P(4)-O(16A)	40.5(19)
O(9)#6-K(1)-O(14)#1	102.2(7)	O(15B)-P(4)-O(15A)	38(2)
O(3)#6-K(1)-O(16B)#1	97.8(9)	O(14)-P(4)-O(15A)	88.2(19)
O(16A)#1-K(1)-O(16B)#1	21.1(10)	O(13)-P(4)-O(15A)	112.2(18)
O(5)-K(1)-O(16B)#1	106.9(9)	O(16B)-P(4)-O(15A)	101(2)
O(13)-K(1)-O(16B)#1	63.9(9)	O(16A)-P(4)-O(15A)	141(2)

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

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

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

#10 -x+1,y+1/2,-z+2   #11 x-1,y+1,z

#12 -x+1,y+1/2,-z+1   #13 -x+2,y+1/2,-z+2

#14 x+1,y+1,z   #15 -x+2,y-1/2,-z+2

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

Table S3b. Selected distances (Å) and angles (deg) for $Li_2RbBi(PO_4)_2$.

Bi(1)-O(10)#1	2.15(2)	O(6)-Rb(1)-O(10)#5	73.6(6)
Bi(1)-O(8)	2.13(3)	O(8)#10-Rb(1)-O(10)#5	72.9(7)
Bi(1)-O(4)#2	2.33(2)	O(1)#11-Rb(1)-O(10)#5	75.9(6)
Bi(1)-O(5)#3	2.35(2)	O(9)#5-Rb(1)-O(10)#5	47.5(6)
Bi(1)-O(11)#4	2.67(2)	O(6)-Rb(1)-O(7)#5	83.3(6)
Bi(2)-O(11)#7	2.34(2)	O(8)#10-Rb(1)-O(7)#5	141.3(7)
Bi(2)-O(11)	2.34(2)	O(1)#11-Rb(1)-O(7)#5	60.5(6)
Bi(2)-O(3)#8	2.37(2)	O(9)#5-Rb(1)-O(7)#5	60.2(6)
Bi(2)-O(3)#9	2.37(2)	O(10)#5-Rb(1)-O(7)#5	107.1(6)
Bi(2)-O(12)#7	2.44(2)	O(6)-Rb(1)-O(6)#2	117.6(7)
Bi(2)-O(12)	2.44(2)	O(8)#10-Rb(1)-O(6)#2	104.5(7)
Bi(2)-O(5)#8	2.64(2)	O(1)#11-Rb(1)-O(6)#2	86.8(6)
Bi(2)-O(5)#9	2.64(2)	O(9)#5-Rb(1)-O(6)#2	123.2(6)
Rb(1)-O(6)	2.77(2)	O(10)#5-Rb(1)-O(6)#2	162.6(6)
Rb(1)-O(8)#10	2.85(3)	O(7)#5-Rb(1)-O(6)#2	63.7(6)
Rb(1)-O(1)#11	2.98(2)	O(6)-Rb(1)-O(4)#2	78.3(6)
Rb(1)-O(9)#5	3.07(2)	O(8)#10-Rb(1)-O(4)#2	118.2(6)
Rb(1)-O(10)#5	3.06(2)	O(1)#11-Rb(1)-O(4)#2	132.0(6)
Rb(1)-O(7)#5	3.07(2)	O(9)#5-Rb(1)-O(4)#2	128.1(6)
Rb(1)-O(6)#2	3.06(2)	O(10)#5-Rb(1)-O(4)#2	148.8(6)
Rb(1)-O(4)#2	3.15(2)	O(7)#5-Rb(1)-O(4)#2	82.4(6)
Rb(1)-O(10)#11	3.41(2)	O(6)#2-Rb(1)-O(4)#2	47.8(6)
Rb(1)-O(8)	3.56(3)	O(6)-Rb(1)-O(10)#11	167.5(6)
Rb(2)-O(3)#3	3.01(2)	O(8)#10-Rb(1)-O(10)#11	55.4(7)
Rb(2)-O(3)	3.01(2)	O(1)#11-Rb(1)-O(10)#11	45.7(6)
Rb(2)-O(11)#2	3.04(2)	O(9)#5-Rb(1)-O(10)#11	104.1(6)
Rb(2)-O(11)#4	3.04(2)	O(10)#5-Rb(1)-O(10)#11	100.8(6)
Rb(2)-O(2)#3	3.05(3)	O(7)#5-Rb(1)-O(10)#11	87.8(6)
Rb(2)-O(2)	3.05(3)	O(6)#2-Rb(1)-O(10)#11	65.3(6)
Rb(2)-O(12)#2	3.20(2)	O(4)#2-Rb(1)-O(10)#11	109.3(6)
Rb(2)-O(12)#4	3.20(2)	O(6)-Rb(1)-O(8)	43.2(6)
Li(1)-O(7)#12	1.84(8)	O(8)#10-Rb(1)-O(8)	105.8(5)
Li(1)-O(6)	1.95(6)	O(1)#11-Rb(1)-O(8)	165.0(6)
Li(1)-O(9)#5	1.98(7)	O(9)#5-Rb(1)-O(8)	105.9(6)
Li(1)-O(4)#5	2.04(7)	O(10)#5-Rb(1)-O(8)	94.9(6)
Li(2)-O(1)#2	1.72(6)	O(7)#5-Rb(1)-O(8)	112.6(6)
Li(2)-O(3)	1.82(6)	O(6)#2-Rb(1)-O(8)	102.3(6)
Li(2)-O(12)	1.99(7)	O(4)#2-Rb(1)-O(8)	54.6(6)
Li(2)-O(5)#7	2.11(6)	Li(3)#5-Rb(1)-O(8)	133.1(12)
Li(3)-O(1)#2	1.81(6)	Li(1)#2-Rb(1)-O(8)	122.5(11)
Li(3)-O(9)	1.95(7)	O(10)#11-Rb(1)-O(8)	149.3(6)
Li(3)-O(2)#3	1.96(6)	O(3)#3-Rb(2)-O(3)	103.5(9)

Li(3)-O(7)	1.98(6)	O(3)#3-Rb(2)-O(11)#2	146.9(6)
P(1)-O(2)	1.46(3)	O(3)-Rb(2)-O(11)#2	65.0(6)
P(1)-O(3)	1.54(2)	O(3)#3-Rb(2)-O(11)#4	65.0(6)
P(1)-O(5)	1.54(2)	O(3)-Rb(2)-O(11)#4	146.9(6)
P(1)-O(11)	1.59(3)	O(11)#2-Rb(2)-O(11)#4	140.8(10)
P(2)-O(6)	1.48(2)	O(3)#3-Rb(2)-O(2)#3	49.0(7)
P(2)-O(7)	1.52(2)	O(3)-Rb(2)-O(2)#3	80.0(6)
P(2)-O(8)	1.53(3)	O(11)#2-Rb(2)-O(2)#3	143.6(7)
P(2)-O(4)	1.55(3)	O(11)#4-Rb(2)-O(2)#3	69.2(7)
P(3)-O(1)	1.49(3)	O(3)#3-Rb(2)-O(2)	80.0(6)
P(3)-O(9)	1.53(3)	O(3)-Rb(2)-O(2)	49.0(7)
P(3)-O(12)	1.56(2)	O(11)#2-Rb(2)-O(2)	69.2(7)
P(3)-O(10)	1.57(2)	O(11)#4-Rb(2)-O(2)	143.6(7)
O(10)#1-Bi(1)-O(8)	87.2(9)	O(2)#3-Rb(2)-O(2)	95.8(10)
O(10)#1-Bi(1)-O(4)#2	94.5(8)	O(3)#3-Rb(2)-O(12)#2	141.4(6)
O(8)-Bi(1)-O(4)#2	88.0(9)	O(3)-Rb(2)-O(12)#2	58.8(6)
O(10)#1-Bi(1)-O(5)#3	87.4(8)	O(11)#2-Rb(2)-O(12)#2	61.3(6)
O(8)-Bi(1)-O(5)#3	90.3(9)	O(11)#4-Rb(2)-O(12)#2	109.7(6)
O(4)#2-Bi(1)-O(5)#3	177.4(9)	O(2)#3-Rb(2)-O(12)#2	92.6(6)
O(10)#1-Bi(1)-O(11)#4	91.5(8)	O(2)-Rb(2)-O(12)#2	103.8(6)
O(8)-Bi(1)-O(11)#4	161.8(9)	O(3)#3-Rb(2)-O(12)#4	58.8(6)
O(4)#2-Bi(1)-O(11)#4	110.2(8)	O(3)-Rb(2)-O(12)#4	141.4(6)
O(5)#3-Bi(1)-O(11)#4	71.5(8)	O(11)#2-Rb(2)-O(12)#4	109.7(6)
O(11)#7-Bi(2)-O(11)	120.0(12)	O(11)#4-Rb(2)-O(12)#4	61.3(6)
O(11)#7-Bi(2)-O(3)#8	140.4(8)	O(2)#3-Rb(2)-O(12)#4	103.8(6)
O(11)-Bi(2)-O(3)#8	87.3(8)	O(2)-Rb(2)-O(12)#4	92.6(6)
O(11)#7-Bi(2)-O(3)#9	87.3(8)	O(12)#2-Rb(2)-O(12)#4	155.4(9)
O(11)-Bi(2)-O(3)#9	140.4(8)	O(7)#12-Li(1)-O(6)	117(4)
O(3)#8-Bi(2)-O(3)#9	87.4(11)	O(7)#12-Li(1)-O(9)#5	114(3)
O(11)#7-Bi(2)-O(12)#7	83.6(8)	O(6)-Li(1)-O(9)#5	104(3)
O(11)-Bi(2)-O(12)#7	76.7(8)	O(7)#12-Li(1)-O(4)#5	105(3)
O(3)#8-Bi(2)-O(12)#7	133.5(7)	O(6)-Li(1)-O(4)#5	115(3)
O(3)#9-Bi(2)-O(12)#7	78.7(7)	O(9)#5-Li(1)-O(4)#5	101(3)
O(11)#7-Bi(2)-O(12)	76.7(8)	O(1)#2-Li(2)-O(3)	121(3)
O(11)-Bi(2)-O(12)	83.6(8)	O(1)#2-Li(2)-O(12)	125(3)
O(3)#8-Bi(2)-O(12)	78.8(7)	O(3)-Li(2)-O(12)	103(3)
O(3)#9-Bi(2)-O(12)	133.5(7)	O(1)#2-Li(2)-O(5)#7	99(3)
O(12)#7-Bi(2)-O(12)	140.1(11)	O(3)-Li(2)-O(5)#7	97(3)
O(11)#7-Bi(2)-O(5)#8	153.1(7)	O(12)-Li(2)-O(5)#7	108(3)
O(11)-Bi(2)-O(5)#8	72.1(8)	O(2)-P(1)-O(3)	113.9(14)
O(3)#8-Bi(2)-O(5)#8	57.6(7)	O(2)-P(1)-O(5)	107.2(14)
O(3)#9-Bi(2)-O(5)#8	72.0(7)	O(3)-P(1)-O(5)	103.9(13)
O(12)#7-Bi(2)-O(5)#8	75.9(7)	O(2)-P(1)-O(11)	111.0(15)
O(12)-Bi(2)-O(5)#8	130.0(7)	O(3)-P(1)-O(11)	111.7(13)

O(11)#7-Bi(2)-O(5)#9	72.1(8)	O(5)-P(1)-O(11)	108.7(15)
O(11)-Bi(2)-O(5)#9	153.1(7)	O(6)-P(2)-O(7)	113.9(13)
O(3)#8-Bi(2)-O(5)#9	72.0(7)	O(6)-P(2)-O(8)	108.2(13)
O(3)#9-Bi(2)-O(5)#9	57.6(7)	O(7)-P(2)-O(8)	104.9(14)
O(12)#7-Bi(2)-O(5)#9	130.0(7)	O(6)-P(2)-O(4)	112.1(14)
O(12)-Bi(2)-O(5)#9	75.9(7)	O(7)-P(2)-O(4)	110.3(13)
O(5)#8-Bi(2)-O(5)#9	108.4(10)	O(8)-P(2)-O(4)	106.9(14)
O(6)-Rb(1)-O(8)#10	130.6(7)	O(1)-P(3)-O(9)	111.5(15)
O(6)-Rb(1)-O(1)#11	121.9(7)	O(1)-P(3)-O(12)	112.4(14)
O(8)#10-Rb(1)-O(1)#11	83.1(7)	O(9)-P(3)-O(12)	112.4(13)
O(6)-Rb(1)-O(9)#5	63.8(6)	O(1)-P(3)-O(10)	110.3(15)
O(8)#10-Rb(1)-O(9)#5	113.4(7)	O(9)-P(3)-O(10)	105.6(13)
O(1)#11-Rb(1)-O(9)#5	59.1(7)	O(12)-P(3)-O(10)	104.2(12)

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

Table S3c. Selected distances (Å) and angles (deg) for $Li_2CsBi(PO_4)_2$.

Cs(1)-O(6)#1	2.94(2)	O(1)#7-Cs(2)-O(1)	142.6(8)
Cs(1)-O(3)	2.973(19)	O(10)#6-Cs(2)-O(4)#3	79.2(5)
Cs(1)-O(6)#2	3.14(2)	O(10)#3-Cs(2)-O(4)#3	47.0(5)
Cs(1)-O(11)#3	3.186(19)	O(1)#7-Cs(2)-O(4)#3	141.4(5)
Cs(1)-O(8)	3.21(2)	O(1)-Cs(2)-O(4)#3	70.1(6)
Cs(1)-O(5)#4	3.23(2)	O(10)#6-Cs(2)-O(4)#6	47.0(5)
Cs(1)-O(12)#2	3.29(2)	O(10)#3-Cs(2)-O(4)#6	79.2(5)
Cs(1)-O(7)#3	3.30(2)	O(1)#7-Cs(2)-O(4)#6	70.1(6)
Cs(1)-O(7)	3.43(2)	O(1)-Cs(2)-O(4)#6	141.4(5)
Cs(1)-O(3)#1	3.501(19)	O(4)#3-Cs(2)-O(4)#6	93.1(7)
Cs(2)-O(10)#6	3.14(2)	O(10)#6-Cs(2)-O(9)#8	138.8(5)
Cs(2)-O(10)#3	3.14(2)	O(10)#3-Cs(2)-O(9)#8	58.4(5)
Cs(2)-O(1)#7	3.14(2)	O(1)#7-Cs(2)-O(9)#8	112.7(5)
Cs(2)-O(1)	3.14(2)	O(1)-Cs(2)-O(9)#8	59.9(5)
Cs(2)-O(4)#3	3.25(2)	O(4)#3-Cs(2)-O(9)#8	102.1(5)
Cs(2)-O(4)#6	3.25(2)	O(4)#6-Cs(2)-O(9)#8	92.2(5)
Cs(2)-O(9)#8	3.244(19)	O(10)#6-Cs(2)-O(9)#9	58.4(5)
Cs(2)-O(9)#9	3.244(19)	O(10)#3-Cs(2)-O(9)#9	138.8(5)
Cs(2)-O(4)	3.70(2)	O(1)#7-Cs(2)-O(9)#9	59.9(5)
Cs(2)-O(4)#7	3.70(2)	O(1)-Cs(2)-O(9)#9	112.7(5)
Bi(1)-O(3)	2.123(19)	O(4)#3-Cs(2)-O(9)#9	92.2(5)
Bi(1)-O(7)	2.149(19)	O(4)#6-Cs(2)-O(9)#9	102.1(5)
Bi(1)-O(12)#10	2.36(2)	O(9)#8-Cs(2)-O(9)#9	159.2(7)
Bi(1)-O(2)#3	2.41(2)	O(10)#6-Cs(2)-O(4)	134.8(5)
Bi(1)-O(1)	2.75(2)	O(10)#3-Cs(2)-O(4)	105.7(5)
Bi(2)-O(1)#8	2.34(2)	O(1)#7-Cs(2)-O(4)	104.2(5)
Bi(2)-O(1)	2.34(2)	O(1)-Cs(2)-O(4)	42.3(5)
Bi(2)-O(10)#3	2.423(19)	O(4)#3-Cs(2)-O(4)	93.9(5)
Bi(2)-O(10)#12	2.423(19)	O(4)#6-Cs(2)-O(4)	173.0(5)
Bi(2)-O(9)	2.485(19)	O(9)#8-Cs(2)-O(4)	86.4(5)
Bi(2)-O(9)#8	2.486(19)	O(9)#9-Cs(2)-O(4)	77.6(5)
Bi(2)-O(2)#3	2.68(2)	O(10)#6-Cs(2)-O(4)#7	105.7(5)
Bi(2)-O(2)#12	2.68(2)	O(10)#3-Cs(2)-O(4)#7	134.8(5)
Li(1)-O(4)	1.87(5)	O(1)#7-Cs(2)-O(4)#7	42.3(5)
Li(1)-O(11)#9	1.96(6)	O(1)-Cs(2)-O(4)#7	104.2(5)
Li(1)-O(8)#13	2.01(5)	O(4)#3-Cs(2)-O(4)#7	173.0(5)
Li(1)-O(5)#10	2.04(6)	O(4)#6-Cs(2)-O(4)#7	93.9(5)
Li(2)-O(8)	1.88(6)	O(9)#8-Cs(2)-O(4)#7	77.6(5)
Li(2)-O(10)#12	1.92(6)	O(9)#9-Cs(2)-O(4)#7	86.4(5)
Li(2)-O(2)#3	1.95(6)	O(4)-Cs(2)-O(4)#7	79.1(6)
Li(2)-O(9)#3	1.96(7)	O(3)-Bi(1)-O(7)	84.2(7)
Li(3)-O(6)	1.84(5)	O(3)-Bi(1)-O(12)#10	89.3(7)

Li(3)-O(12)#11	1.99(5)	O(7)-Bi(1)-O(12)#10	97.9(8)
Li(3)-O(11)#1	2.05(5)	O(3)-Bi(1)-O(2)#3	90.0(7)
Li(3)-O(5)#15	2.05(6)	O(7)-Bi(1)-O(2)#3	84.4(7)
P(1)-O(4)	1.51(2)	O(12)#10-Bi(1)-O(2)#3	177.5(7)
P(1)-O(10)	1.54(2)	O(3)-Bi(1)-O(1)	163.5(7)
P(1)-O(2)	1.56(2)	O(7)-Bi(1)-O(1)	93.2(7)
P(1)-O(1)	1.57(2)	O(12)#10-Bi(1)-O(1)	107.2(7)
P(2)-O(6)	1.49(2)	O(2)#3-Bi(1)-O(1)	73.5(6)
P(2)-O(5)	1.54(2)	O(1)#8-Bi(2)-O(1)	115.7(11)
P(2)-O(12)	1.55(2)	O(1)#8-Bi(2)-O(10)#3	142.9(7)
P(2)-O(3)	1.596(19)	O(1)-Bi(2)-O(10)#3	88.3(7)
P(3)-O(8)	1.50(2)	O(1)#8-Bi(2)-O(10)#12	88.3(7)
P(3)-O(11)	1.53(2)	O(1)-Bi(2)-O(10)#12	142.9(7)
P(3)-O(7)	1.55(2)	O(10)#3-Bi(2)-O(10)#12	87.8(9)
P(3)-O(9)	1.55(2)	O(1)#8-Bi(2)-O(9)	82.6(7)
O(6)#1-Cs(1)-O(3)	135.3(6)	O(1)-Bi(2)-O(9)	77.1(7)
O(6)#1-Cs(1)-O(6)#2	113.5(6)	O(10)#3-Bi(2)-O(9)	132.3(7)
O(3)-Cs(1)-O(6)#2	107.7(5)	O(10)#12-Bi(2)-O(9)	78.7(6)
O(6)#1-Cs(1)-O(11)#3	63.6(5)	O(1)#8-Bi(2)-O(9)#8	77.1(7)
O(3)-Cs(1)-O(11)#3	109.4(5)	O(1)-Bi(2)-O(9)#8	82.6(7)
O(6)#2-Cs(1)-O(11)#3	119.9(5)	O(10)#3-Bi(2)-O(9)#8	78.7(6)
O(6)#1-Cs(1)-O(8)	118.7(5)	O(10)#12-Bi(2)-O(9)#8	132.3(7)
O(3)-Cs(1)-O(8)	80.2(5)	O(9)-Bi(2)-O(9)#8	141.4(9)
O(6)#2-Cs(1)-O(8)	85.8(5)	O(1)#8-Bi(2)-O(2)#3	151.9(7)
O(11)#3-Cs(1)-O(8)	56.8(5)	O(1)-Bi(2)-O(2)#3	76.0(7)
O(6)#1-Cs(1)-O(5)#4	81.3(6)	O(10)#3-Bi(2)-O(2)#3	57.3(7)
O(3)-Cs(1)-O(5)#4	136.2(5)	O(10)#12-Bi(2)-O(2)#3	71.0(7)
O(6)#2-Cs(1)-O(5)#4	60.4(5)	O(9)-Bi(2)-O(2)#3	75.1(6)
O(11)#3-Cs(1)-O(5)#4	59.9(5)	O(9)#8-Bi(2)-O(2)#3	130.9(6)
O(8)-Cs(1)-O(5)#4	58.0(5)	O(1)#8-Bi(2)-O(2)#12	76.0(7)
O(6)#1-Cs(1)-O(12)#2	77.8(5)	O(1)-Bi(2)-O(2)#12	151.9(7)
O(3)-Cs(1)-O(12)#2	123.5(5)	O(10)#3-Bi(2)-O(2)#12	71.0(7)
O(6)#2-Cs(1)-O(12)#2	46.1(5)	O(10)#12-Bi(2)-O(2)#12	57.3(7)
O(11)#3-Cs(1)-O(12)#2	127.2(5)	O(9)-Bi(2)-O(2)#12	130.9(6)
O(8)-Cs(1)-O(12)#2	129.2(5)	O(9)#8-Bi(2)-O(2)#12	75.1(6)
O(5)#4-Cs(1)-O(12)#2	80.6(5)	O(2)#3-Bi(2)-O(2)#12	106.2(9)
O(6)#1-Cs(1)-O(7)#3	73.7(5)	O(4)-Li(1)-O(11)#9	130(3)
O(3)-Cs(1)-O(7)#3	73.3(5)	O(4)-Li(1)-O(8)#13	114(3)
O(6)#2-Cs(1)-O(7)#3	160.5(5)	O(11)#9-Li(1)-O(8)#13	100(2)
O(11)#3-Cs(1)-O(7)#3	45.3(5)	O(4)-Li(1)-O(5)#10	103(2)
O(8)-Cs(1)-O(7)#3	75.1(5)	O(11)#9-Li(1)-O(5)#10	106(2)
O(5)#4-Cs(1)-O(7)#3	104.8(5)	O(8)#13-Li(1)-O(5)#10	101(2)
O(12)#2-Cs(1)-O(7)#3	149.6(5)	O(6)-Li(3)-O(12)#11	122(3)
O(6)#1-Cs(1)-O(7)	162.2(5)	O(6)-Li(3)-O(11)#1	112(3)

O(3)-Cs(1)-O(7)	52.5(5)	O(12)#11-Li(3)-O(11)#1	104(2)
O(6)#2-Cs(1)-O(7)	69.5(5)	O(6)-Li(3)-O(5)#15	111(3)
O(11)#3-Cs(1)-O(7)	99.2(5)	O(12)#11-Li(3)-O(5)#15	100(2)
O(8)-Cs(1)-O(7)	43.5(5)	O(11)#1-Li(3)-O(5)#15	106(2)
O(5)#4-Cs(1)-O(7)	85.7(5)	O(4)-P(1)-O(10)	113.1(12)
O(12)#2-Cs(1)-O(7)	112.2(5)	O(4)-P(1)-O(2)	110.7(12)
O(7)#3-Cs(1)-O(7)	98.2(5)	O(10)-P(1)-O(2)	105.1(12)
O(6)#1-Cs(1)-O(3)#1	44.2(5)	O(4)-P(1)-O(1)	110.0(12)
O(3)-Cs(1)-O(3)#1	111.8(4)	O(10)-P(1)-O(1)	109.6(12)
O(6)#2-Cs(1)-O(3)#1	101.3(5)	O(2)-P(1)-O(1)	108.1(13)
O(11)#3-Cs(1)-O(3)#1	106.5(5)	O(6)-P(2)-O(5)	114.7(12)
O(8)-Cs(1)-O(3)#1	162.8(5)	O(6)-P(2)-O(12)	111.7(13)
O(5)#4-Cs(1)-O(3)#1	111.9(5)	O(5)-P(2)-O(12)	111.2(13)
O(12)#2-Cs(1)-O(3)#1	55.2(5)	O(6)-P(2)-O(3)	106.6(12)
O(7)#3-Cs(1)-O(3)#1	96.0(5)	O(5)-P(2)-O(3)	104.0(12)
O(7)-Cs(1)-O(3)#1	153.7(4)	O(12)-P(2)-O(3)	108.1(11)
Li(3)#1-Cs(1)-O(3)#1	75.8(9)	O(8)-P(3)-O(11)	111.2(13)
O(10)#6-Cs(2)-O(10)#3	101.5(7)	O(8)-P(3)-O(7)	108.0(12)
O(10)#6-Cs(2)-O(1)#7	63.8(5)	O(11)-P(3)-O(7)	108.1(11)
O(10)#3-Cs(2)-O(1)#7	147.9(6)	O(8)-P(3)-O(9)	110.6(13)
O(10)#6-Cs(2)-O(1)	147.9(6)	O(11)-P(3)-O(9)	111.7(12)
O(10)#3-Cs(2)-O(1)	63.8(5)	O(7)-P(3)-O(9)	107.1(11)

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

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

#6 -x+1,y-1,-z   #7 -x+1,y,-z   #8 -x+1,y,-z+1

#9 x,y,z-1   #10 x,y+1,z   #11 -x+1/2,y+1/2,-z

#12 -x+1,y-1,-z+1   #13 x,y+1,z-1   #14 -x+1/2,y+3/2,-z

#15 -x+1/2,y-1/2,-z   #16 -x+1/2,y-3/2,-z

#17 -x+1,y+1,-z+1