Inorganic Chemistry Frontiers

Supporting Information

$ACs_5Bi_4(PO_4)_2(P_2O_7)_3$ (A = K, Rb and Cs) with two kinds of isolated P−O groups designed by dimensional reduction theory

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Table S1. Crystal data and structure refinement for $ACs_5Bi_4(PO_4)_2(P_2O_7)_3$ (A = K, Rb and Cs).

	$KCs_5Bi_4(PO_4)_2(P_2O_7)_3$	$RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$	$Cs_6Bi_4(PO_4)_2(P_2O_7)_3$
Formula weight	2251.33	2297.70	2345.14
Temperature / K	298(2)	299(2)	299(2)
Wavelength / Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group, Z	$P2_1/c$, 4	$P2_1/c$, 4	$P2_1/c$, 4
a / Å	9.1435(4)	9.1839(9)	9.1860(7)
b / Å	9.3581(4)	9.3584(9)	9.3662(8)
c / Å	36.4405(18)	36.724(3)	37.368(3)
β / °	95.9210(10)	96.100(3)	96.677(2)
Volume / $Å^3$	3101.4(2)	3138.5(5)	3193.3(4)
ρ / Mg/m^3	4.822	4.863	4.878
μ / mm^{-1}	29.067	30.132	29.224
$F(000)$	3912	3984	4056
Crystal size / mm^3	0.090x0.083x0.075	0.082x0.080x0.063	0.120x0.068x0.077
Θ range for data collection / °	2.24 to 27.54	2.23 to 27.50	2.19 to 27.53
Limiting indices	$-11\le h\le 11$, $-12\le k\le 12$, $-47\le l\le 47$	$-11\le h\le 11$, $-12\le k\le 12$, $-47\le l\le 35$	$-11\le h\le 11$, $-12\le k\le 12$, $-48\le l\le 48$
Reflections collected / unique	39188 / 7124 [R(int) = 0.0578]	32088 / 7181 [R(int) = 0.0815]	35551 / 7318 [R(int) = 0.0952]
Completeness	99.8%	99.9 %	99.7 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7124 / 0 / 425	7181 / 0 / 279	7318 / 0 / 279
Goodness-of-fit on F^2	1.042	1.057	1.080
Final R indices [$F_o^2>2\sigma(F_o^2)$] [a]	R_1 = 0.0361, wR_2 = 0.0787	R_1 = 0.0508, wR_2 = 0.1021	R_1 = 0.0489, wR_2 = 0.0893
R indices (all data) [a]	R_1 = 0.0481, wR_2 = 0.0854	R_1 = 0.0818, wR_2 = 0.1187	R_1 = 0.0838, wR_2 = 0.1051
Largest diff. peak and hole / $e\cdot Å^{-3}$	1.579 and -4.415	2.499 and -4.728	2.362 and -2.539

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

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$.

Atom	x	y	z	U(eq) [a]	BVS
Bi(1)	-0.3231(1)	1.1217(1)	0.0516(1)	0.012(1)	2.95
Bi(2)	-0.0724(1)	0.6221(1)	0.1892(1)	0.015(1)	3.29
Bi(3)	0.5579(1)	0.7927(1)	0.1228(1)	0.012(1)	2.86
Bi(4)	-0.1338(1)	1.5913(1)	0.0542(1)	0.014(1)	2.98
K(1)	0.0539(3)	1.2926(3)	0.1239(1)	0.019(1)	1.14
Cs(1)	0.1775(1)	0.9975(1)	0.0496(1)	0.022(1)	1.07
Cs(2)	0.4017(1)	0.4559(1)	0.1889(1)	0.027(1)	1.14
Cs(3)	-0.6421(1)	1.4815(1)	0.0506(1)	0.037(1)	1.37
Cs(4)	0.2334(1)	0.6359(1)	0.3007(1)	0.034(1)	1.13
Cs(5)	0.2665(1)	0.9759(1)	0.2001(1)	0.031(1)	0.98
P(1)	0.5599(3)	0.7972(3)	0.0247(1)	0.011(1)	5.03
P(2)	-0.0950(3)	0.8948(3)	0.1205(1)	0.014(1)	5.21
P(3)	0.6207(3)	0.7357(3)	0.2248(1)	0.016(1)	4.96
P(4)	0.4591(3)	1.1677(3)	0.1190(1)	0.012(1)	5.04
P(5)	-0.0435(3)	1.3046(3)	0.0178(1)	0.013(1)	4.98
P(6)	0.1680(3)	0.7074(3)	01268(1)	0.018(1)	5.31
P(7)	0.6804(3)	0.4064(3)	0.1203(1)	0.016(1)	4.95
P(8)	0.9025(3)	0.8410(3)	0.2610(1)	0.019(1)	5.03
O(1)	0.1038(15)	0.5983(14)	0.1021(5)	0.081(5)	2.00
O(2)	0.5822(9)	0.2824(8)	0.1357(2)	0.019(2)	2.34
O(3)	0.6538(8)	0.6613(8)	0.0276(2)	0.015(2)	2.27
O(4)	0.4450(8)	1.1832(8)	0.0775(2)	0.019(2)	2.04
O(5)	0.4350(8)	0.7640(8)	-0.0058(2)	0.015(2)	2.20
O(6)	-0.1278(8)	1.1646(8)	0.0237(2)	0.018(2)	2.28
O(7)	-0.1521(8)	1.4304(8)	0.0103(2)	0.018(2)	2.27
O(8)	0.4931(9)	0.8250(9)	0.0609(2)	0.022(2)	2.00
O(9)	0.6485(9)	0.9264(8)	0.0144(2)	0.020(2)	2.09
O(10)	0.0292(9)	1.2724(8)	-0.0180(3)	0.025(2)	2.21
O(11)	0.7225(10)	0.3594(10)	0.0825(2)	0.028(2)	2.00
O(12)	0.7184(9)	0.6072(9)	0.2178(3)	0.025(2)	2.08
O(13)	0.7370(9)	0.8572(8)	0.2412(3)	0.024(2)	2.31
O(14)	0.0627(10)	1.3389(10)	0.0508(2)	0.030(2)	1.86
O(15)	0.5310(11)	1.0274(9)	0.1319(3)	0.037(2)	2.11
O(16)	0.0752(9)	0.8250(10)	0.1200(3)	0.033(2)	2.27
O(17)	0.5170(10)	0.7078(10)	0.2530(3)	0.029(2)	1.80
O(18)	-0.0068(9)	0.7793(9)	0.2319(2)	0.024(2)	2.20
O(19)	0.5495(9)	0.7962(10)	0.1889(2)	0.028(2)	1.95
O(20)	0.8103(10)	0.4181(11)	0.1491(3)	0.037(2)	1.91
O(21)	-0.1828(12)	0.8190(14)	0.0897(3)	0.058(4)	1.86
O(22)	0.3201(9)	0.7545(12)	0.2955(3)	0.036(2)	2.20
O(23)	0.3255(10)	1.1998(12)	0.1375(3)	0.037(2)	1.98

O(24)	0.9039(10)	0.7567(12)	0.2955(3)	0.036(2)	1.90
O(25)	0.5829(13)	0.5382(9)	0.1172(3)	0.043(3)	2.00
O(26)	0.9455(11)	0.9965(10)	0.2673(3)	0.039(3)	2.20
O(27)	0.1596(11)	0.6762(12)	0.1676(3)	0.045(3)	2.17
O(28)	-0.1008(11)	1.0528(10)	0.1162(4)	0.049(3)	1.84
O(29)	-0.1443(12)	0.8386(13)	0.1560(3)	0.052(3)	1.96

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

Table S3. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$.

Atom	x	y	z	U(eq) [a]	BVS
Bi(1)	0.6772(1)	0.8739(1)	1.0514(1)	0.012(1)	2.83
Bi(2)	1.0735(1)	0.6306(1)	0.8109(1)	0.016(1)	3.24
Bi(3)	0.4407(1)	0.7895(1)	0.8776(1)	0.012(1)	3.15
Bi(4)	0.1283(1)	0.5881(1)	0.9455(1)	0.014(1)	3.16
Rb(1)	1.0605(2)	0.7077(2)	1.1244(1)	0.020(1)	1.15
Cs(1)	0.5953(1)	0.4560(1)	0.8108(1)	0.028(1)	0.97
Cs(2)	0.8179(1)	0.9999(1)	0.9510(1)	0.025(1)	1.09
Cs(3)	0.3596(1)	0.5210(1)	1.0490(1)	0.036(1)	1.44
Cs(4)	0.7309(1)	0.9701(1)	0.7991(1)	0.033(1)	0.96
Cs(5)	0.2336(2)	1.1330(1)	0.8000(1)	0.038(1)	1.08
P(1)	0.9036(5)	0.3400(5)	0.7621(1)	0.021(1)	4.93
P(2)	0.9554(5)	0.6973(4)	1.0166(1)	0.013(1)	4.97
P(3)	0.3762(5)	0.7373(5)	0.7749(1)	0.017(1)	5.08
P(4)	0.5315(5)	0.1645(4)	0.8798(1)	0.014(1)	5.07
P(5)	1.0944(5)	0.8938(4)	0.8801(1)	0.014(1)	5.10
P(6)	0.8303(5)	0.7111(5)	0.8745(1)	0.017(1)	5.39
P(7)	0.3232(5)	0.4112(4)	0.8797(1)	0.015(1)	5.01
P(8)	0.4364(5)	0.7956(4)	0.9741(1)	0.013(1)	4.96
O(1)	0.8703(12)	0.8369(12)	1.0232(3)	0.016(2)	2.26
O(2)	0.3411(12)	0.6609(12)	0.9718(3)	0.017(2)	2.24
O(3)	0.5595(12)	0.7644(12)	1.0054(3)	0.020(3)	2.15
O(4)	0.8487(12)	0.5716(12)	1.0104(3)	0.017(2)	2.30
O(5)	0.2807(14)	0.6089(13)	0.7813(3)	0.027(3)	2.08
O(6)	0.2623(13)	0.8565(13)	0.7580(3)	0.025(3)	2.34
O(7)	0.4063(12)	0.2784(12)	0.8641(3)	0.020(3)	2.34
O(8)	0.2764(13)	0.3676(13)	0.9166(3)	0.026(3)	1.84
O(9)	1.0663(14)	0.6629(14)	1.0482(3)	0.030(3)	1.89
O(10)	0.3471(13)	0.9262(13)	0.9832(3)	0.022(3)	2.08
O(11)	0.1938(14)	0.4364(14)	0.8516(3)	0.032(3)	1.88
O(12)	0.5586(14)	0.1873(14)	0.9204(3)	0.028(3)	2.01
O(13)	0.9259(14)	0.8545(14)	0.8828(3)	0.030(3)	2.24
O(14)	0.5049(13)	0.8208(13)	0.9382(3)	0.026(3)	2.02
O(15)	0.4830(14)	0.7098(14)	0.7480(3)	0.029(3)	1.81
O(16)	0.6790(15)	0.7670(15)	0.8779(4)	0.034(3)	2.27
O(17)	0.4315(15)	0.5338(14)	0.8828(4)	0.033(3)	2.04
O(18)	1.0246(13)	0.7293(13)	0.9802(3)	0.024(3)	2.17
O(19)	0.6593(15)	0.1897(15)	0.8592(4)	0.038(3)	1.85
O(20)	1.1327(18)	0.8561(17)	0.8425(4)	0.050(4)	1.87
O(21)	0.9960(13)	0.2860(13)	0.7325(3)	0.022(3)	2.18
O(22)	0.9054(15)	0.2500(15)	0.7950(4)	0.035(3)	1.96
O(23)	0.4440(14)	0.8000(14)	0.8107(4)	0.033(3)	1.93

O(24)	0.8460(15)	0.6706(15)	0.8360(4)	0.037(3)	2.11
O(25)	0.4529(16)	0.0236(15)	0.8708(4)	0.039(4)	2.12
O(26)	0.8815(18)	0.6063(17)	0.9017(4)	0.051(4)	2.03
O(27)	1.1116(18)	1.0452(18)	0.8920(4)	0.054(4)	1.82
O(28)	1.1863(19)	0.7940(19)	0.9062(5)	0.058(5)	1.83
O(29)	0.9458(16)	0.4965(16)	0.7705(4)	0.043(4)	2.14

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

Table S4. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$.

Atom	x	y	z	U(eq) [a]	BVS
Bi(1)	-0.0767(1)	0.6434(1)	0.1889(1)	0.013(1)	3.08
Bi(2)	-0.3155(1)	0.1294(1)	0.0519(1)	0.013(1)	2.98
Bi(3)	-0.1209(1)	0.5835(1)	0.0553(1)	0.012(1)	3.05
Bi(4)	0.5636(1)	0.7922(1)	0.1229(1)	0.011(1)	3.21
Cs(1)	0.4086(1)	0.4615(1)	0.1894(1)	0.024(1)	0.92
Cs(2)	-0.6324(1)	0.4799(1)	0.0484(1)	0.023(1)	1.31
Cs(3)	0.0713(1)	0.2818(1)	0.1248(1)	0.029(1)	1.21
Cs(4)	-0.8091(1)	0.0019(1)	0.0478(1)	0.023(1)	1.03
Cs(5)	0.2685(1)	0.9659(1)	0.2021(1)	0.028(1)	0.97
Cs(6)	0.2390(1)	0.6341(1)	0.2972(1)	0.030(1)	1.14
P(1)	-0.0925(4)	-0.1055(4)	0.1182(1)	0.014(1)	5.04
P(2)	-0.0471(4)	0.3032(4)	0.0160(1)	0.013(1)	4.90
P(3)	0.6871(4)	0.4203(4)	0.1228(1)	0.013(1)	5.01
P(4)	0.6295(4)	0.7446(5)	0.2256(1)	0.017(1)	5.01
P(5)	0.0898(4)	0.3411(4)	0.2357(1)	0.016(1)	4.86
P(6)	0.1730(4)	0.7130(4)	0.1249(1)	0.016(1)	5.09
P(7)	-0.4288(4)	0.7978(4)	0.0284(1)	0.012(1)	4.92
P(8)	0.4835(4)	0.1663(4)	0.1219(1)	0.015(1)	5.17
O(1)	-0.1295(10)	0.1612(11)	0.0230(3)	0.017(2)	2.28
O(2)	0.0004(10)	0.2941(11)	0.2658(3)	0.018(2)	2.07
O(3)	-0.3340(10)	0.6618(11)	0.0305(3)	0.016(2)	2.19
O(4)	-0.3323(11)	0.9277(12)	0.0223(3)	0.023(3)	2.17
O(5)	0.7357(11)	0.3841(11)	0.0863(3)	0.023(2)	1.82
O(6)	0.0643(11)	0.3402(12)	0.0475(3)	0.026(3)	1.83
O(7)	0.0522(11)	0.4975(12)	0.2251(3)	0.024(3)	2.12
O(8)	-0.1592(10)	0.4264(11)	0.0114(3)	0.019(2)	2.24
O(9)	-0.5049(10)	0.8167(11)	0.0634(3)	0.018(2)	1.98
O(10)	0.2582(11)	0.3620(11)	0.2546(3)	0.023(3)	2.29
O(11)	-0.5491(11)	0.7807(11)	-0.0030(3)	0.023(3)	2.04
O(12)	0.0169(11)	0.2750(11)	-0.0200(3)	0.023(3)	2.10
O(13)	0.5716(11)	0.5341(12)	0.1205(3)	0.024(3)	2.05
O(14)	0.5136(11)	0.7187(12)	0.2494(3)	0.027(3)	1.79
O(15)	0.8136(12)	0.4474(13)	0.1516(3)	0.032(3)	1.92
O(16)	0.0858(11)	0.2417(12)	0.2048(3)	0.030(3)	1.96
O(17)	-0.1170(11)	0.0310(12)	0.0975(3)	0.028(3)	1.93
O(18)	0.6107(11)	0.2800(12)	0.1374(3)	0.024(3)	2.17
O(19)	0.1451(11)	0.6724(13)	0.1632(3)	0.030(3)	1.97
O(20)	0.3268(12)	0.7727(13)	0.1249(3)	0.032(3)	2.15
O(21)	0.8143(12)	0.7713(13)	0.1011(3)	0.035(3)	1.84
O(22)	0.0756(11)	0.8534(12)	0.1137(3)	0.024(3)	2.17
O(23)	0.1326(13)	0.6025(14)	0.0980(3)	0.044(3)	1.96

O(24)	0.7247(11)	0.6137(12)	0.2212(3)	0.029(3)	2.04
O(25)	0.5722(13)	0.0281(13)	0.1253(3)	0.038(3)	2.08
O(26)	-0.1085(14)	-0.1014(14)	0.1574(4)	0.046(4)	1.77
O(27)	0.3742(14)	0.1755(16)	0.1468(4)	0.054(4)	2.10
O(28)	0.4388(12)	0.1955(14)	0.0827(3)	0.038(3)	1.94
O(29)	0.5777(12)	0.8122(13)	0.1895(3)	0.038(3)	1.87

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

Table S5. Bond lengths (Å) and angles (°) for $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$.

K(1)-O(23)	2.630(10)	Cs(4)-O(2)#7	3.047(8)
K(1)-O(28)	2.653(10)	Cs(4)-O(13)#4	3.050(9)
K(1)-O(14)	2.709(9)	Cs(4)-O(26)#4	3.113(11)
K(1)-O(20)#3	2.757(10)	Cs(4)-O(24)#2	3.205(9)
K(1)-O(24)#7	2.943(10)	Cs(4)-O(15)#4	3.258(10)
K(1)-O(1)#9	3.016(15)	Cs(4)-O(20)#7	3.260(11)
K(1)-O(11)#3	3.302(10)	Cs(4)-O(17)	3.336(9)
Cs(1)-O(9)#12	3.041(8)	Cs(4)-O(29)#13	3.341(12)
Cs(1)-O(6)#1	3.066(8)	Cs(4)-O(18)	3.432(9)
Cs(1)-O(4)	3.086(8)	Cs(4)-O(28)#13	3.465(13)
Cs(1)-O(16)	3.133(10)	Cs(5)-O(24)#7	3.068(10)
Cs(1)-O(6)	3.254(8)	Cs(5)-O(19)	3.147(9)
Cs(1)-O(10)#1	3.291(8)	Cs(5)-O(27)	3.159(13)
Cs(1)-O(8)	3.295(8)	Cs(5)-O(23)	3.185(11)
Cs(1)-O(14)	3.365(10)	Cs(5)-O(12)#7	3.223(9)
Cs(1)-O(22)	3.606(10)	Cs(5)-O(17)#7	3.293(9)
Cs(2)-O(27)	3.066(10)	Cs(5)-O(18)	3.402(9)
Cs(2)-O(23)#5	3.078(10)	Cs(5)-O(16)	3.444(10)
Cs(2)-O(13)#4	3.099(9)	Cs(5)-O(22)	3.615(11)
Cs(2)-O(2)	3.127(8)	Cs(5)-O(15)	3.675(12)
Cs(2)-O(17)#4	3.176(10)	Bi(1)-O(5)#1	2.149(7)
Cs(2)-O(12)	3.297(8)	Bi(1)-O(6)	2.179(7)
Cs(2)-O(25)	3.327(11)	Bi(1)-O(9)#2	2.273(8)
Cs(2)-O(17)	3.409(10)	Bi(1)-O(4)#2	2.478(8)
Cs(2)-O(24)#4	3.455(10)	Bi(1)-O(11)#3	2.508(9)
Cs(2)-O(19)	3.459(10)	Bi(3)-O(22)	2.198(9)
Cs(3)-O(7)#10	2.879(8)	Bi(3)-O(15)	2.239(8)
Cs(3)-O(14)#2	3.012(9)	Bi(3)-O(8)	2.292(8)
Cs(3)-O(4)#2	3.038(8)	Bi(3)-O(25)	2.403(9)
Cs(3)-O(25)#3	3.061(12)	Bi(3)-O(19)	2.421(9)
Cs(3)-O(3)#1	3.141(8)	Bi(4)-O(10)#8	2.132(8)
Cs(3)-O(1)#3	3.320(16)	Bi(4)-O(3)#3	2.180(7)
Cs(3)-O(3)#3	3.364(8)	Bi(4)-O(7)	2.192(8)
Cs(3)-O(8)#3	3.450(9)	Bi(4)-O(21)#9	2.556(11)
Cs(3)-O(5)#3	3.466(8)	Bi(4)-O(1)#9	2.643(13)
Cs(3)-O(5)#1	3.487(8)	P(1)-O(9)	1.523(8)
Cs(3)-O(11)#3	3.602(9)	P(1)-O(8)	1.531(8)
Bi(2)-O(18)	2.180(8)	P(1)-O(3)	1.532(8)
Bi(2)-O(26)#4	2.204(9)	P(1)-O(5)	1.542(7)
Bi(2)-O(12)#2	2.275(9)	P(2)-O(28)	1.487(10)
Bi(2)-O(27)	2.392(10)	P(2)-O(21)	1.489(10)
Bi(2)-O(29)	2.417(10)	P(2)-O(29)	1.506(10)
Bi(2)-O(20)#2	2.571(9)	P(2)-O(16)	1.609(8)

P(3)-O(17)	1.492(9)	P(4)-O(23)	1.485(9)
P(3)-O(19)	1.508(9)	P(4)-O(4)	1.510(8)
P(3)-O(12)	1.535(9)	P(4)-O(15)	1.520(9)
P(3)-O(13)	1.629(8)	P(4)-O(2)#9	1.627(8)
P(5)-O(14)	1.499(9)	P(6)-O(1)	1.444(13)
P(5)-O(7)	1.546(8)	P(6)-O(22)	1.492(9)
P(5)-O(6)	1.547(8)	P(6)-O(27)	1.526(10)
P(5)-O(10)	1.554(9)	P(6)-O(16)	1.603(9)
P(7)-O(20)	1.506(10)	P(8)-O(24)	1.482(10)
P(7)-O(25)	1.519(9)	P(8)-O(26)	1.519(9)
P(7)-O(11)	1.532(9)	P(8)-O(18)#11	1.526(9)
P(7)-O(2)	1.604(8)	P(8)-O(13)	1.615(8)
O(23)-K(1)-O(28)	102.9(3)	O(9)#12-Cs(1)-O(6)#1	59.3(2)
O(23)-K(1)-O(14)	96.6(3)	O(9)#12-Cs(1)-O(4)	70.2(2)
O(28)-K(1)-O(14)	95.8(4)	O(6)#1-Cs(1)-O(4)	127.4(2)
O(23)-K(1)-O(20)#3	149.0(3)	O(9)#12-Cs(1)-O(16)	162.7(2)
O(28)-K(1)-O(20)#3	87.5(3)	O(6)#1-Cs(1)-O(16)	118.0(2)
O(14)-K(1)-O(20)#3	111.5(3)	O(4)-Cs(1)-O(16)	105.5(2)
O(23)-K(1)-O(24)#7	75.5(3)	O(9)#12-Cs(1)-O(6)	99.6(2)
O(28)-K(1)-O(24)#7	91.3(4)	O(6)#1-Cs(1)-O(6)	86.6(2)
O(14)-K(1)-O(24)#7	170.5(3)	O(4)-Cs(1)-O(6)	116.9(2)
O(20)#3-K(1)-O(24)#7	75.1(3)	O(16)-Cs(1)-O(6)	97.2(2)
O(23)-K(1)-O(1)#9	101.4(4)	O(9)#12-Cs(1)-O(10)#1	103.8(2)
O(28)-K(1)-O(1)#9	150.3(4)	O(6)#1-Cs(1)-O(10)#1	44.5(2)
O(14)-K(1)-O(1)#9	64.5(4)	O(4)-Cs(1)-O(10)#1	162.7(2)
O(20)#3-K(1)-O(1)#9	80.4(4)	O(16)-Cs(1)-O(10)#1	75.2(2)
O(24)#7-K(1)-O(1)#9	111.3(4)	O(6)-Cs(1)-O(10)#1	79.8(2)
O(23)-K(1)-O(11)#3	162.3(3)	O(9)#12-Cs(1)-O(8)	71.9(2)
O(28)-K(1)-O(11)#3	70.0(3)	O(6)#1-Cs(1)-O(8)	85.1(2)
O(14)-K(1)-O(11)#3	68.8(3)	O(4)-Cs(1)-O(8)	65.2(2)
O(20)#3-K(1)-O(11)#3	48.5(3)	O(16)-Cs(1)-O(8)	91.0(2)
O(24)#7-K(1)-O(11)#3	119.8(2)	O(6)-Cs(1)-O(8)	170.4(2)
O(1)#9-K(1)-O(11)#3	81.8(3)	O(10)#1-Cs(1)-O(8)	97.6(2)
O(27)-Cs(2)-O(23)#5	104.9(3)	O(9)#12-Cs(1)-O(14)	88.6(2)
O(27)-Cs(2)-O(13)#4	93.6(2)	O(6)#1-Cs(1)-O(14)	117.6(2)
O(23)#5-Cs(2)-O(13)#4	100.5(2)	O(4)-Cs(1)-O(14)	72.5(2)
O(27)-Cs(2)-O(2)	127.3(3)	O(16)-Cs(1)-O(14)	106.4(2)
O(23)#5-Cs(2)-O(2)	47.1(2)	O(6)-Cs(1)-O(14)	44.58(19)
O(13)#4-Cs(2)-O(2)	129.9(2)	O(10)#1-Cs(1)-O(14)	124.4(2)
O(27)-Cs(2)-O(17)#4	140.6(2)	O(8)-Cs(1)-O(14)	137.2(2)
O(23)#5-Cs(2)-O(17)#4	81.9(3)	O(9)#12-Cs(1)-O(22)	121.7(2)
O(13)#4-Cs(2)-O(17)#4	47.4(2)	O(6)#1-Cs(1)-O(22)	109.2(2)
O(2)-Cs(2)-O(17)#4	86.1(2)	O(4)-Cs(1)-O(22)	84.3(2)

O(27)-Cs(2)-O(12)	112.3(3)	O(16)-Cs(1)-O(22)	41.3(2)
O(23)#5-Cs(2)-O(12)	131.7(2)	O(6)-Cs(1)-O(22)	138.4(2)
O(13)#4-Cs(2)-O(12)	106.6(2)	O(10)#1-Cs(1)-O(22)	85.5(2)
O(2)-Cs(2)-O(12)	85.3(2)	O(8)-Cs(1)-O(22)	49.8(2)
O(17)#4-Cs(2)-O(12)	87.9(2)	O(14)-Cs(1)-O(22)	132.8(2)
O(27)-Cs(2)-O(25)	92.9(2)	O(7)#10-Cs(3)-O(14)#2	67.3(2)
O(23)#5-Cs(2)-O(25)	78.6(3)	O(7)#10-Cs(3)-O(4)#2	129.9(2)
O(13)#4-Cs(2)-O(25)	173.5(2)	O(14)#2-Cs(3)-O(4)#2	78.3(2)
O(2)-Cs(2)-O(25)	45.2(2)	O(7)#10-Cs(3)-O(25)#3	153.4(2)
O(17)#4-Cs(2)-O(25)	126.2(2)	O(14)#2-Cs(3)-O(25)#3	127.2(3)
O(12)-Cs(2)-O(25)	70.1(3)	O(4)#2-Cs(3)-O(25)#3	76.8(2)
O(27)-Cs(2)-O(17)	82.7(3)	O(7)#10-Cs(3)-O(3)#1	57.6(2)
O(23)#5-Cs(2)-O(17)	172.1(3)	O(14)#2-Cs(3)-O(3)#1	82.3(2)
O(13)#4-Cs(2)-O(17)	76.5(2)	O(4)#2-Cs(3)-O(3)#1	83.4(2)
O(2)-Cs(2)-O(17)	129.7(2)	O(25)#3-Cs(3)-O(3)#1	138.6(2)
O(17)#4-Cs(2)-O(17)	90.83(3)	O(7)#10-Cs(3)-O(1)#3	84.4(3)
O(12)-Cs(2)-O(17)	44.3(2)	O(14)#2-Cs(3)-O(1)#3	57.7(3)
O(25)-Cs(2)-O(17)	103.6(2)	O(4)#2-Cs(3)-O(1)#3	107.2(3)
O(27)-Cs(2)-O(24)#4	80.2(3)	O(25)#3-Cs(3)-O(1)#3	87.0(3)
O(23)#5-Cs(2)-O(24)#4	62.9(2)	O(3)#1-Cs(3)-O(1)#3	133.9(3)
O(13)#4-Cs(2)-O(24)#4	45.4(2)	O(7)#10-Cs(3)-O(3)#3	98.3(2)
O(2)-Cs(2)-O(24)#4	108.0(2)	O(14)#2-Cs(3)-O(3)#3	165.0(2)
O(17)#4-Cs(2)-O(24)#4	68.5(2)	O(4)#2-Cs(3)-O(3)#3	110.4(2)
O(12)-Cs(2)-O(24)#4	151.4(2)	O(25)#3-Cs(3)-O(3)#3	67.6(2)
O(25)-Cs(2)-O(24)#4	137.0(3)	O(3)#1-Cs(3)-O(3)#3	86.56(19)
O(17)-Cs(2)-O(24)#4	117.3(2)	O(1)#3-Cs(3)-O(3)#3	127.1(3)
O(27)-Cs(2)-O(19)	69.7(3)	O(7)#10-Cs(3)-O(8)#3	90.9(2)
O(2)#7-Cs(4)-O(13)#4	134.1(2)	O(14)#2-Cs(3)-O(8)#3	136.4(2)
O(2)#7-Cs(4)-O(26)#4	176.7(2)	O(4)#2-Cs(3)-O(8)#3	137.92(19)
O(13)#4-Cs(4)-O(26)#4	46.2(2)	O(25)#3-Cs(3)-O(8)#3	63.2(2)
O(2)#7-Cs(4)-O(24)#2	109.3(2)	O(3)#1-Cs(3)-O(8)#3	118.24(19)
O(13)#4-Cs(4)-O(24)#2	113.8(2)	O(1)#3-Cs(3)-O(8)#3	84.0(3)
O(26)#4-Cs(4)-O(24)#2	71.7(3)	O(3)#3-Cs(3)-O(8)#3	43.34(18)
O(2)#7-Cs(4)-O(15)#4	45.3(2)	O(7)#10-Cs(3)-O(5)#3	58.72(19)
O(13)#4-Cs(4)-O(15)#4	91.5(2)	O(14)#2-Cs(3)-O(5)#3	125.2(2)
O(26)#4-Cs(4)-O(15)#4	136.2(2)	O(4)#2-Cs(3)-O(5)#3	146.1(2)
O(24)#2-Cs(4)-O(15)#4	134.4(3)	O(25)#3-Cs(3)-O(5)#3	100.2(2)
O(2)#7-Cs(4)-O(20)#7	45.5(2)	O(3)#1-Cs(3)-O(5)#3	77.04(19)
O(13)#4-Cs(4)-O(20)#7	175.1(2)	O(1)#3-Cs(3)-O(5)#3	106.4(3)
O(26)#4-Cs(4)-O(20)#7	134.6(2)	O(3)#3-Cs(3)-O(5)#3	41.67(17)
O(24)#2-Cs(4)-O(20)#7	65.1(2)	O(8)#3-Cs(3)-O(5)#3	42.38(18)
O(15)#4-Cs(4)-O(20)#7	86.5(2)	O(7)#10-Cs(3)-O(5)#1	99.88(19)
O(2)#7-Cs(4)-O(17)	84.6(2)	O(14)#2-Cs(3)-O(5)#1	103.8(2)
O(2)#7-Cs(4)-O(13)#4	134.1(2)	O(4)#2-Cs(3)-O(5)#1	53.8(2)

O(2)#7-Cs(4)-O(26)#4	176.7(2)	O(25)#3-Cs(3)-O(5)#1	97.6(2)
O(13)#4-Cs(4)-O(26)#4	46.2(2)	O(3)#1-Cs(3)-O(5)#1	42.63(17)
O(2)#7-Cs(4)-O(24)#2	109.3(2)	O(1)#3-Cs(3)-O(5)#1	158.0(3)
O(13)#4-Cs(4)-O(24)#2	113.8(2)	O(3)#3-Cs(3)-O(5)#1	73.97(18)
O(26)#4-Cs(4)-O(24)#2	71.7(3)	O(8)#3-Cs(3)-O(5)#1	117.31(18)
O(2)#7-Cs(4)-O(15)#4	45.3(2)	O(5)#3-Cs(3)-O(5)#1	94.10(17)
O(13)#4-Cs(4)-O(15)#4	91.5(2)	O(7)#10-Cs(3)-O(11)#3	148.1(2)
O(26)#4-Cs(4)-O(15)#4	136.2(2)	O(14)#2-Cs(3)-O(11)#3	131.2(2)
O(24)#2-Cs(4)-O(15)#4	134.4(3)	O(4)#2-Cs(3)-O(11)#3	53.2(2)
O(13)#4-Cs(4)-O(17)	78.3(2)	O(25)#3-Cs(3)-O(11)#3	43.6(2)
O(26)#4-Cs(4)-O(17)	92.4(3)	O(3)#1-Cs(3)-O(11)#3	95.82(19)
O(24)#2-Cs(4)-O(17)	132.4(2)	O(1)#3-Cs(3)-O(11)#3	126.9(3)
O(15)#4-Cs(4)-O(17)	88.1(3)	O(3)#3-Cs(3)-O(11)#3	59.83(18)
O(20)#7-Cs(4)-O(17)	106.0(2)	O(8)#3-Cs(3)-O(11)#3	87.22(19)
O(2)#7-Cs(4)-O(29)#13	99.1(2)	O(5)#3-Cs(3)-O(11)#3	101.26(18)
O(13)#4-Cs(4)-O(29)#13	64.1(2)	O(5)#1-Cs(3)-O(11)#3	54.02(18)
O(26)#4-Cs(4)-O(29)#13	83.9(3)	O(24)#7-Cs(5)-O(19)	153.3(3)
O(24)#2-Cs(4)-O(29)#13	92.8(3)	O(24)#7-Cs(5)-O(27)	129.8(3)
O(15)#4-Cs(4)-O(29)#13	63.8(3)	O(19)-Cs(5)-O(27)	72.8(2)
O(20)#7-Cs(4)-O(29)#13	111.1(2)	O(24)#7-Cs(5)-O(23)	66.3(3)
O(17)-Cs(4)-O(29)#13	130.9(3)	O(19)-Cs(5)-O(23)	93.2(2)
O(2)#7-Cs(4)-O(18)	129.9(2)	O(27)-Cs(5)-O(23)	112.6(3)
O(13)#4-Cs(4)-O(18)	92.9(2)	O(24)#7-Cs(5)-O(12)#7	66.3(2)
O(26)#4-Cs(4)-O(18)	48.5(2)	O(19)-Cs(5)-O(12)#7	111.5(2)
O(24)#2-Cs(4)-O(18)	44.9(2)	O(27)-Cs(5)-O(12)#7	131.9(2)
O(15)#4-Cs(4)-O(18)	175.2(2)	O(23)-Cs(5)-O(12)#7	114.8(2)
O(20)#7-Cs(4)-O(18)	89.3(2)	O(24)#7-Cs(5)-O(17)#7	71.9(2)
O(17)-Cs(4)-O(18)	90.8(2)	O(19)-Cs(5)-O(17)#7	87.8(2)
O(29)#13-Cs(4)-O(18)	120.1(2)	O(27)-Cs(5)-O(17)#7	157.7(2)
O(2)#7-Cs(4)-O(28)#13	69.7(2)	O(23)-Cs(5)-O(17)#7	78.5(2)
O(13)#4-Cs(4)-O(28)#13	107.7(2)	O(12)#7-Cs(5)-O(17)#7	45.7(2)
O(26)#4-Cs(4)-O(28)#13	113.6(3)	O(24)#7-Cs(5)-O(18)	92.9(2)
O(24)#2-Cs(4)-O(28)#13	73.7(2)	O(19)-Cs(5)-O(18)	113.5(2)
O(15)#4-Cs(4)-O(28)#13	62.3(3)	O(27)-Cs(5)-O(18)	55.8(2)
O(20)#7-Cs(4)-O(28)#13	67.5(2)	O(23)-Cs(5)-O(18)	141.7(2)
O(17)-Cs(4)-O(28)#13	149.5(2)	O(12)#7-Cs(5)-O(18)	81.5(2)
O(29)#13-Cs(4)-O(28)#13	43.6(2)	O(17)#7-Cs(5)-O(18)	127.1(2)
O(18)-Cs(4)-O(28)#13	118.1(2)	O(24)#7-Cs(5)-O(16)	96.7(2)
O(5)#1-Bi(1)-O(6)	84.0(3)	O(19)-Cs(5)-O(16)	93.6(2)
O(5)#1-Bi(1)-O(9)#2	85.5(3)	O(27)-Cs(5)-O(16)	43.4(2)
O(6)-Bi(1)-O(9)#2	85.4(3)	O(23)-Cs(5)-O(16)	73.9(2)
O(5)#1-Bi(1)-O(4)#2	79.8(3)	O(12)#7-Cs(5)-O(16)	152.1(2)
O(6)-Bi(1)-O(4)#2	155.4(3)	O(17)#7-Cs(5)-O(16)	152.4(2)
O(9)#2-Bi(1)-O(4)#2	111.4(3)	O(18)-Cs(5)-O(16)	77.3(2)

O(5)#1-Bi(1)-O(11)#3	87.2(3)	O(24)#7-Cs(5)-O(22)	130.1(2)
O(6)-Bi(1)-O(11)#3	86.5(3)	O(19)-Cs(5)-O(22)	53.9(2)
O(9)#2-Bi(1)-O(11)#3	169.6(3)	O(27)-Cs(5)-O(22)	41.9(2)
O(4)#2-Bi(1)-O(11)#3	74.4(3)	O(23)-Cs(5)-O(22)	76.2(2)
O(18)-Bi(2)-O(26)#4	76.2(4)	O(12)#7-Cs(5)-O(22)	163.6(2)
O(18)-Bi(2)-O(12)#2	84.1(3)	O(17)#7-Cs(5)-O(22)	131.8(2)
O(26)#4-Bi(2)-O(12)#2	92.5(4)	O(18)-Cs(5)-O(22)	97.2(2)
O(18)-Bi(2)-O(27)	84.5(4)	O(16)-Cs(5)-O(22)	39.9(2)
O(26)#4-Bi(2)-O(27)	86.0(4)	O(24)#7-Cs(5)-O(15)	107.2(2)
O(12)#2-Bi(2)-O(27)	168.5(4)	O(19)-Cs(5)-O(15)	51.4(2)
O(18)-Bi(2)-O(29)	80.4(4)	O(27)-Cs(5)-O(15)	93.6(2)
O(26)#4-Bi(2)-O(29)	154.6(4)	O(23)-Cs(5)-O(15)	42.0(2)
O(12)#2-Bi(2)-O(29)	94.8(3)	O(12)#7-Cs(5)-O(15)	127.6(2)
O(27)-Bi(2)-O(29)	82.1(3)	O(17)#7-Cs(5)-O(15)	82.1(2)
O(18)-Bi(2)-O(20)#2	167.2(3)	O(18)-Cs(5)-O(15)	149.3(2)
O(26)#4-Bi(2)-O(20)#2	99.8(4)	O(16)-Cs(5)-O(15)	77.5(2)
O(12)#2-Bi(2)-O(20)#2	83.9(3)	O(22)-Cs(5)-O(15)	52.1(2)
O(27)-Bi(2)-O(20)#2	107.6(4)	O(9)-P(1)-O(8)	110.3(5)
O(29)-Bi(2)-O(20)#2	105.2(4)	O(9)-P(1)-O(3)	111.6(4)
O(26)#4-Bi(2)-O(12)#2	92.5(4)	O(8)-P(1)-O(3)	110.6(5)
O(22)-Bi(3)-O(15)	92.3(4)	O(9)-P(1)-O(5)	110.8(5)
O(22)-Bi(3)-O(8)	81.0(3)	O(8)-P(1)-O(5)	108.9(4)
O(15)-Bi(3)-O(8)	89.7(3)	O(3)-P(1)-O(5)	104.5(4)
O(22)-Bi(3)-O(25)	86.5(4)	O(28)-P(2)-O(21)	112.5(7)
O(15)-Bi(3)-O(25)	176.1(4)	O(28)-P(2)-O(29)	115.4(7)
O(8)-Bi(3)-O(25)	93.7(3)	O(21)-P(2)-O(29)	107.1(8)
O(22)-Bi(3)-O(19)	83.9(3)	O(28)-P(2)-O(16)	105.7(5)
O(15)-Bi(3)-O(19)	79.9(4)	O(21)-P(2)-O(16)	108.7(6)
O(8)-Bi(3)-O(19)	161.3(3)	O(29)-P(2)-O(16)	107.3(6)
O(25)-Bi(3)-O(19)	96.4(3)	O(17)-P(3)-O(19)	114.5(5)
O(10)#8-Bi(4)-O(3)#3	88.9(3)	O(17)-P(3)-O(12)	113.5(5)
O(10)#8-Bi(4)-O(7)	87.9(3)	O(19)-P(3)-O(12)	110.9(5)
O(3)#3-Bi(4)-O(7)	83.4(3)	O(17)-P(3)-O(13)	107.8(5)
O(10)#8-Bi(4)-O(21)#9	85.9(4)	O(19)-P(3)-O(13)	105.3(5)
O(3)#3-Bi(4)-O(21)#9	77.3(3)	O(12)-P(3)-O(13)	103.8(4)
O(7)-Bi(4)-O(21)#9	159.8(3)	O(23)-P(4)-O(4)	116.4(5)
O(10)#8-Bi(4)-O(1)#9	90.2(5)	O(23)-P(4)-O(15)	112.6(6)
O(3)#3-Bi(4)-O(1)#9	156.9(3)	O(4)-P(4)-O(15)	112.4(5)
O(7)-Bi(4)-O(1)#9	119.7(4)	O(23)-P(4)-O(2)#9	105.4(5)
O(21)#9-Bi(4)-O(1)#9	79.6(4)	O(4)-P(4)-O(2)#9	107.1(4)
O(1)-P(6)-O(22)	116.7(8)	O(15)-P(4)-O(2)#9	101.2(5)
O(1)-P(6)-O(27)	114.4(9)	O(14)-P(5)-O(7)	109.3(5)
O(22)-P(6)-O(27)	109.2(6)	O(14)-P(5)-O(6)	111.1(5)
O(1)-P(6)-O(16)	109.0(7)	O(7)-P(5)-O(6)	110.4(4)

O(22)-P(6)-O(16)	102.5(5)	O(14)-P(5)-O(10)	114.6(5)
O(27)-P(6)-O(16)	103.4(6)	O(7)-P(5)-O(10)	108.8(5)
O(20)-P(7)-O(25)	114.0(6)	O(6)-P(5)-O(10)	102.4(4)
O(20)-P(7)-O(11)	113.2(5)	O(24)-P(8)-O(26)	113.8(6)
O(25)-P(7)-O(11)	111.5(6)	O(24)-P(8)-O(18)#11	115.5(6)
O(20)-P(7)-O(2)	103.8(5)	O(26)-P(8)-O(18)#11	108.5(6)
O(25)-P(7)-O(2)	105.5(5)	O(24)-P(8)-O(13)	110.8(5)
O(11)-P(7)-O(2)	108.0(5)	O(26)-P(8)-O(13)	101.1(5)
		O(18)#11-P(8)-O(13)	106.0(5)

Symmetry transformations used to generate equivalent atoms:

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

Table S6. Bond lengths (Å) and angles (°) for $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$.

Bi(1)-O(3)	2.164(11)	Cs(1)-O(19)	3.080(14)
Bi(1)-O(1)	2.174(11)	Cs(1)-O(6)#6	3.110(12)
Bi(1)-O(10)#1	2.260(12)	Cs(1)-O(24)	3.120(14)
Bi(1)-O(8)#2	2.562(12)	Cs(1)-O(15)#6	3.188(13)
Bi(1)-O(12)#2	2.564(13)	Cs(1)-O(7)	3.214(12)
Bi(2)-O(29)	2.187(15)	Cs(1)-O(17)	3.260(13)
Bi(2)-O(21)#3	2.201(12)	Cs(1)-O(5)	3.302(12)
Bi(2)-O(5)#4	2.297(13)	Cs(1)-O(15)	3.394(13)
Bi(2)-O(24)	2.401(14)	Cs(2)-O(1)	3.051(11)
Bi(2)-O(20)	2.442(16)	Cs(2)-O(10)#1	3.062(12)
Bi(2)-O(11)#4	2.532(13)	Cs(2)-O(12)#7	3.073(13)
Bi(3)-O(16)	2.198(14)	Cs(2)-O(13)	3.105(13)
Bi(3)-O(25)#7	2.208(15)	Cs(2)-O(18)	3.277(12)
Bi(3)-O(14)	2.261(12)	Cs(2)-O(1)#10	3.294(11)
Bi(3)-O(17)	2.403(14)	Cs(2)-O(14)	3.318(13)
Bi(3)-O(23)	2.461(13)	Cs(2)-O(9)#10	3.329(13)
Bi(3)-O(28)#8	2.662(17)	Cs(2)-O(16)	3.588(13)
Bi(4)-O(18)#8	2.130(12)	Cs(3)-O(4)#2	2.878(11)
Bi(4)-O(2)	2.195(11)	Cs(3)-O(9)#8	3.001(13)
Bi(4)-O(4)#2	2.198(11)	Cs(3)-O(12)#2	3.017(13)
Bi(4)-O(28)#8	2.498(18)	Cs(3)-O(17)#2	3.033(13)
Bi(4)-O(26)#8	2.641(16)	Cs(3)-O(2)	3.109(11)
Bi(4)-O(8)	2.745(12)	Cs(3)-O(26)#2	3.234(16)
Rb(1)-O(19)#5	2.753(15)	Cs(3)-O(2)#2	3.389(11)
Rb(1)-O(27)#10	2.830(17)	Cs(3)-O(3)	3.427(12)
Rb(1)-O(9)	2.836(13)	Cs(3)-O(14)#2	3.446(12)
Rb(1)-O(11)#2	2.914(14)	Cs(3)-O(3)#2	3.463(12)
Rb(1)-O(22)#5	2.968(13)	Cs(3)-O(8)#2	3.600(13)
Rb(1)-O(26)#5	3.154(16)	Cs(4)-O(22)#7	3.083(14)
Rb(1)-O(8)#2	3.369(13)	Cs(4)-O(19)#7	3.136(14)
P(1)-O(22)	1.474(14)	Cs(4)-O(23)	3.147(14)
P(1)-O(21)	1.533(12)	Cs(4)-O(5)#11	3.217(12)
P(1)-O(29)	1.538(16)	Cs(4)-O(24)	3.242(14)
P(1)-O(6)#6	1.628(13)	Cs(4)-O(15)#11	3.341(13)
P(2)-O(9)	1.495(13)	Cs(4)-O(21)#3	3.350(12)
P(2)-O(4)	1.532(12)	Cs(4)-O(16)	3.537(13)
P(2)-O(1)	1.555(11)	Cs(4)-O(13)	3.560(13)
P(2)-O(18)	1.568(12)	Cs(4)-O(15)	3.704(13)
P(3)-O(15)	1.486(14)	Cs(5)-O(7)#7	3.021(11)
P(3)-O(23)	1.511(14)	Cs(5)-O(6)	3.037(12)
P(3)-O(5)	1.521(13)	Cs(5)-O(29)#11	3.183(15)
P(3)-O(6)	1.608(13)	Cs(5)-O(22)#12	3.194(14)
P(4)-O(19)	1.481(15)	Cs(5)-O(20)#8	3.213(16)

P(4)-O(12)	1.502(13)	Cs(5)-O(25)#7	3.280(14)
P(4)-O(25)	1.523(15)	Cs(5)-O(15)#11	3.373(13)
P(4)-O(7)	1.627(12)	Cs(5)-O(21)#12	3.435(12)
P(5)-O(27)	1.485(17)	Cs(5)-O(11)#7	3.455(13)
P(5)-O(20)	1.503(16)	Cs(5)-O(23)	3.666(13)
P(5)-O(28)	1.526(17)	P(7)-O(11)	1.507(14)
P(5)-O(13)	1.604(14)	P(7)-O(17)	1.515(14)
P(6)-O(26)	1.442(16)	P(7)-O(8)	1.522(13)
P(6)-O(24)	1.487(14)	P(7)-O(7)	1.596(12)
P(6)-O(16)	1.502(14)	P(8)-O(10)	1.528(12)
P(6)-O(13)	1.615(14)	P(8)-O(2)	1.533(12)
		P(8)-O(14)	1.539(13)
O(3)-Bi(1)-O(1)	85.3(4)	P(8)-O(3)	1.551(12)
O(3)-Bi(1)-O(10)#1	86.7(4)	O(29)-Bi(2)-O(21)#3	78.2(5)
O(1)-Bi(1)-O(10)#1	84.3(4)	O(29)-Bi(2)-O(5)#4	92.3(5)
O(3)-Bi(1)-O(8)#2	89.1(4)	O(21)#3-Bi(2)-O(5)#4	84.7(4)
O(1)-Bi(1)-O(8)#2	88.5(4)	O(29)-Bi(2)-O(24)	85.6(5)
O(10)#1-Bi(1)-O(8)#2	171.9(4)	O(21)#3-Bi(2)-O(24)	88.7(5)
O(3)-Bi(1)-O(12)#2	80.6(4)	O(5)#4-Bi(2)-O(24)	173.4(5)
O(1)-Bi(1)-O(12)#2	157.5(4)	O(29)-Bi(2)-O(20)	153.5(5)
O(10)#1-Bi(1)-O(12)#2	112.0(4)	O(21)#3-Bi(2)-O(20)	78.8(5)
O(8)#2-Bi(1)-O(12)#2	74.0(4)	O(5)#4-Bi(2)-O(20)	98.5(5)
O(16)-Bi(3)-O(25)#7	91.9(5)	O(24)-Bi(2)-O(20)	80.9(5)
O(16)-Bi(3)-O(14)	81.5(5)	O(29)-Bi(2)-O(11)#4	99.1(5)
O(25)#7-Bi(3)-O(14)	88.4(5)	O(21)#3-Bi(2)-O(11)#4	167.6(4)
O(16)-Bi(3)-O(17)	87.0(5)	O(5)#4-Bi(2)-O(11)#4	83.3(4)
O(25)#7-Bi(3)-O(17)	177.8(5)	O(24)-Bi(2)-O(11)#4	103.2(4)
O(14)-Bi(3)-O(17)	93.3(4)	O(20)-Bi(2)-O(11)#4	106.1(5)
O(16)-Bi(3)-O(23)	83.7(5)	O(18)#8-Bi(4)-O(2)	88.7(4)
O(25)#7-Bi(3)-O(23)	80.9(5)	O(18)#8-Bi(4)-O(4)#2	89.7(4)
O(14)-Bi(3)-O(23)	161.4(5)	O(2)-Bi(4)-O(4)#2	82.8(4)
O(17)-Bi(3)-O(23)	97.1(4)	O(18)#8-Bi(4)-O(28)#8	90.2(5)
O(16)-Bi(3)-O(28)#8	156.2(5)	O(2)-Bi(4)-O(28)#8	77.3(5)
O(25)#7-Bi(3)-O(28)#8	95.0(5)	O(4)#2-Bi(4)-O(28)#8	160.1(5)
O(14)-Bi(3)-O(28)#8	75.9(5)	O(18)#8-Bi(4)-O(26)#8	85.2(5)
O(17)-Bi(3)-O(28)#8	86.8(5)	O(2)-Bi(4)-O(26)#8	156.1(5)
O(23)-Bi(3)-O(28)#8	119.9(5)	O(4)#2-Bi(4)-O(26)#8	120.1(5)
O(19)#5-Rb(1)-O(27)#10	104.5(5)	O(28)#8-Bi(4)-O(26)#8	79.7(5)
O(19)#5-Rb(1)-O(9)	98.8(4)	O(18)#8-Bi(4)-O(8)	165.6(4)
O(27)#10-Rb(1)-O(9)	88.8(4)	O(2)-Bi(4)-O(8)	87.1(4)
O(19)#5-Rb(1)-O(11)#2	148.9(4)	O(4)#2-Bi(4)-O(8)	76.1(4)
O(27)#10-Rb(1)-O(11)#2	89.7(4)	O(28)#8-Bi(4)-O(8)	102.2(5)
O(9)-Rb(1)-O(11)#2	109.3(4)	O(26)#8-Bi(4)-O(8)	104.0(4)
O(19)#5-Rb(1)-O(22)#5	74.8(4)	O(19)-Cs(1)-O(6)#6	98.9(3)

O(27)#10-Rb(1)-O(22)#5	95.8(4)	O(19)-Cs(1)-O(24)	105.1(4)
O(9)-Rb(1)-O(22)#5	172.9(4)	O(6)#6-Cs(1)-O(24)	94.2(3)
O(11)#2-Rb(1)-O(22)#5	76.3(4)	O(19)-Cs(1)-O(15)#6	79.7(4)
O(19)#5-Rb(1)-O(26)#5	102.0(4)	O(6)#6-Cs(1)-O(15)#6	46.9(3)
O(27)#10-Rb(1)-O(26)#5	143.7(5)	O(24)-Cs(1)-O(15)#6	140.5(4)
O(9)-Rb(1)-O(26)#5	62.7(4)	O(19)-Cs(1)-O(7)	46.6(3)
O(11)#2-Rb(1)-O(26)#5	80.0(4)	O(6)#6-Cs(1)-O(7)	129.9(3)
O(22)#5-Rb(1)-O(26)#5	115.1(4)	O(24)-Cs(1)-O(7)	125.6(3)
O(19)#5-Rb(1)-O(8)#2	164.5(4)	O(15)#6-Cs(1)-O(7)	86.7(3)
O(27)#10-Rb(1)-O(8)#2	67.1(4)	O(19)-Cs(1)-O(17)	77.9(4)
O(9)-Rb(1)-O(8)#2	68.9(3)	O(6)#6-Cs(1)-O(17)	175.1(3)
O(11)#2-Rb(1)-O(8)#2	46.4(3)	O(24)-Cs(1)-O(17)	90.3(4)
O(22)#5-Rb(1)-O(8)#2	117.9(3)	O(15)#6-Cs(1)-O(17)	128.4(3)
O(26)#5-Rb(1)-O(8)#2	81.1(4)	O(7)-Cs(1)-O(17)	45.2(3)
O(1)-Cs(2)-O(10)#1	58.3(3)	O(19)-Cs(1)-O(5)	130.3(4)
O(1)-Cs(2)-O(12)#7	130.4(3)	O(6)#6-Cs(1)-O(5)	107.0(3)
O(10)#1-Cs(2)-O(12)#7	74.4(3)	O(24)-Cs(1)-O(5)	114.2(3)
O(1)-Cs(2)-O(13)	116.6(3)	O(15)#6-Cs(1)-O(5)	88.0(3)
O(10)#1-Cs(2)-O(13)	164.2(3)	O(7)-Cs(1)-O(5)	85.0(3)
O(12)#7-Cs(2)-O(13)	104.8(3)	O(17)-Cs(1)-O(5)	72.9(3)
O(1)-Cs(2)-O(18)	45.3(3)	O(19)-Cs(1)-O(15)	169.6(4)
O(10)#1-Cs(2)-O(18)	103.6(3)	O(6)#6-Cs(1)-O(15)	77.4(3)
O(12)#7-Cs(2)-O(18)	163.8(3)	O(24)-Cs(1)-O(15)	85.0(3)
O(13)-Cs(2)-O(18)	72.6(3)	O(15)#6-Cs(1)-O(15)	90.85(4)
O(1)-Cs(2)-O(1)#10	86.0(3)	O(7)-Cs(1)-O(15)	129.1(3)
O(10)#1-Cs(2)-O(1)#10	99.0(3)	O(17)-Cs(1)-O(15)	105.1(3)
O(12)#7-Cs(2)-O(1)#10	117.2(3)	O(5)-Cs(1)-O(15)	44.1(3)
O(13)-Cs(2)-O(1)#10	95.3(3)	O(4)#2-Cs(3)-O(9)#8	66.5(3)
O(18)-Cs(2)-O(1)#10	79.0(3)	O(4)#2-Cs(3)-O(12)#2	132.4(3)
O(1)-Cs(2)-O(14)	85.7(3)	O(9)#8-Cs(3)-O(12)#2	77.9(4)
O(10)#1-Cs(2)-O(14)	74.5(3)	O(4)#2-Cs(3)-O(17)#2	152.4(3)
O(12)#7-Cs(2)-O(14)	67.1(3)	O(9)#8-Cs(3)-O(17)#2	124.8(4)
O(13)-Cs(2)-O(14)	90.6(3)	O(12)#2-Cs(3)-O(17)#2	74.6(4)
O(18)-Cs(2)-O(14)	96.8(3)	O(4)#2-Cs(3)-O(2)	57.9(3)
O(1)#10-Cs(2)-O(14)	171.3(3)	O(9)#8-Cs(3)-O(2)	80.9(3)
O(1)-Cs(2)-O(9)#10	116.5(3)	O(12)#2-Cs(3)-O(2)	86.9(3)
O(10)#1-Cs(2)-O(9)#10	87.9(3)	O(17)#2-Cs(3)-O(2)	142.4(3)
O(12)#7-Cs(2)-O(9)#10	72.3(3)	O(4)#2-Cs(3)-O(26)#2	82.8(4)
O(13)-Cs(2)-O(9)#10	107.1(3)	O(9)#8-Cs(3)-O(26)#2	60.1(4)
O(18)-Cs(2)-O(9)#10	123.8(3)	O(12)#2-Cs(3)-O(26)#2	106.4(4)
O(1)#10-Cs(2)-O(9)#10	44.9(3)	O(17)#2-Cs(3)-O(26)#2	83.4(4)
O(14)-Cs(2)-O(9)#10	138.7(3)	O(2)-Cs(3)-O(26)#2	133.7(4)
O(1)-Cs(2)-O(16)	110.9(3)	O(4)#2-Cs(3)-O(2)#2	99.6(3)
O(10)#1-Cs(2)-O(16)	124.1(3)	O(9)#8-Cs(3)-O(2)#2	165.7(3)

O(12)#7-Cs(2)-O(16)	82.7(3)	O(12)#2-Cs(3)-O(2)#2	111.3(3)
O(13)-Cs(2)-O(16)	41.2(3)	O(17)#2-Cs(3)-O(2)#2	69.2(3)
O(18)-Cs(2)-O(16)	85.6(3)	O(2)-Cs(3)-O(2)#2	88.5(3)
O(1)#10-Cs(2)-O(16)	136.6(3)	O(26)#2-Cs(3)-O(2)#2	124.2(3)
O(14)-Cs(2)-O(16)	49.7(3)	O(4)#2-Cs(3)-O(3)	101.1(3)
O(9)#10-Cs(2)-O(16)	132.1(3)	O(9)#8-Cs(3)-O(3)	103.1(3)
O(22)#7-Cs(4)-O(19)#7	68.0(4)	O(12)#2-Cs(3)-O(3)	56.5(3)
O(22)#7-Cs(4)-O(23)	152.1(4)	O(17)#2-Cs(3)-O(3)	100.1(3)
O(19)#7-Cs(4)-O(23)	89.7(4)	O(2)-Cs(3)-O(3)	43.5(3)
O(22)#7-Cs(4)-O(5)#11	65.1(3)	O(26)#2-Cs(3)-O(3)	159.9(4)
O(19)#7-Cs(4)-O(5)#11	113.1(3)	O(2)#2-Cs(3)-O(3)	75.0(3)
O(23)-Cs(4)-O(5)#11	112.5(3)	O(4)#2-Cs(3)-O(14)#2	91.4(3)
O(22)#7-Cs(4)-O(24)	127.4(4)	O(9)#8-Cs(3)-O(14)#2	136.3(3)
O(19)#7-Cs(4)-O(24)	110.8(4)	O(12)#2-Cs(3)-O(14)#2	135.8(3)
O(23)-Cs(4)-O(24)	75.3(4)	O(17)#2-Cs(3)-O(14)#2	62.8(3)
O(5)#11-Cs(4)-O(24)	135.3(3)	O(2)-Cs(3)-O(14)#2	120.0(3)
O(22)#7-Cs(4)-O(15)#11	71.6(3)	O(26)#2-Cs(3)-O(14)#2	80.8(4)
O(19)#7-Cs(4)-O(15)#11	76.6(3)	O(2)#2-Cs(3)-O(14)#2	43.5(3)
O(23)-Cs(4)-O(15)#11	87.4(3)	O(3)-Cs(3)-O(14)#2	118.5(3)
O(5)#11-Cs(4)-O(15)#11	45.0(3)	O(4)#2-Cs(3)-O(3)#2	59.8(3)
O(24)-Cs(4)-O(15)#11	160.9(3)	O(9)#8-Cs(3)-O(3)#2	125.7(3)
O(22)#7-Cs(4)-O(21)#3	90.5(3)	O(12)#2-Cs(3)-O(3)#2	148.5(3)
O(19)#7-Cs(4)-O(21)#3	143.2(3)	O(17)#2-Cs(3)-O(3)#2	101.0(3)
O(23)-Cs(4)-O(21)#3	117.1(3)	O(2)-Cs(3)-O(3)#2	78.1(3)
O(5)#11-Cs(4)-O(21)#3	81.0(3)	O(26)#2-Cs(3)-O(3)#2	103.9(4)
O(24)-Cs(4)-O(21)#3	58.5(3)	O(2)#2-Cs(3)-O(3)#2	41.7(3)
O(15)#11-Cs(4)-O(21)#3	125.9(3)	O(3)-Cs(3)-O(3)#2	94.9(3)
O(22)#7-Cs(4)-O(16)	127.7(3)	O(14)#2-Cs(3)-O(3)#2	42.8(3)
O(19)#7-Cs(4)-O(16)	73.7(3)	O(4)#2-Cs(3)-O(8)#2	150.5(3)
O(23)-Cs(4)-O(16)	55.2(3)	O(9)#8-Cs(3)-O(8)#2	132.4(3)
O(5)#11-Cs(4)-O(16)	166.8(3)	O(12)#2-Cs(3)-O(8)#2	54.7(3)
O(24)-Cs(4)-O(16)	42.2(3)	O(17)#2-Cs(3)-O(8)#2	43.7(3)
O(15)#11-Cs(4)-O(16)	131.4(3)	O(2)-Cs(3)-O(8)#2	99.0(3)
O(21)#3-Cs(4)-O(16)	100.2(3)	O(26)#2-Cs(3)-O(8)#2	125.2(4)
O(22)#7-Cs(4)-O(13)	94.8(3)	O(2)#2-Cs(3)-O(8)#2	58.6(3)
O(19)#7-Cs(4)-O(13)	73.4(3)	O(3)-Cs(3)-O(8)#2	56.5(3)
O(23)-Cs(4)-O(13)	94.6(3)	O(14)#2-Cs(3)-O(8)#2	85.0(3)
O(5)#11-Cs(4)-O(13)	151.7(3)	O(3)#2-Cs(3)-O(8)#2	100.2(3)
O(24)-Cs(4)-O(13)	42.6(3)	O(7)#7-Cs(5)-O(6)	135.5(3)
O(15)#11-Cs(4)-O(13)	150.0(3)	O(7)#7-Cs(5)-O(29)#11	176.6(4)
O(21)#3-Cs(4)-O(13)	79.4(3)	O(6)-Cs(5)-O(29)#11	46.5(4)
O(16)-Cs(4)-O(13)	39.5(3)	O(7)#7-Cs(5)-O(22)#12	107.7(3)
O(22)#7-Cs(4)-O(15)	146.0(3)	O(6)-Cs(5)-O(22)#12	113.3(3)
O(19)#7-Cs(4)-O(15)	128.6(3)	O(29)#11-Cs(5)-O(22)#12	71.8(4)

O(23)-Cs(4)-O(15)	42.0(3)	O(7)#7-Cs(5)-O(20)#8	98.0(4)
O(5)#11-Cs(4)-O(15)	80.9(3)	O(6)-Cs(5)-O(20)#8	66.7(4)
O(24)-Cs(4)-O(15)	78.4(3)	O(29)#11-Cs(5)-O(20)#8	85.4(4)
O(15)#11-Cs(4)-O(15)	83.32(4)	O(22)#12-Cs(5)-O(20)#8	89.1(4)
O(21)#3-Cs(4)-O(15)	86.0(3)	O(7)#7-Cs(5)-O(25)#7	45.2(3)
O(16)-Cs(4)-O(15)	86.1(3)	O(6)-Cs(5)-O(25)#7	93.3(3)
O(13)-Cs(4)-O(15)	117.6(3)	O(29)#11-Cs(5)-O(25)#7	137.8(4)
O(22)-P(1)-O(21)	115.8(8)	O(22)#12-Cs(5)-O(25)#7	130.4(3)
O(22)-P(1)-O(29)	113.5(8)	O(20)#8-Cs(5)-O(25)#7	63.1(4)
O(21)-P(1)-O(29)	108.0(8)	O(7)#7-Cs(5)-O(15)#11	86.6(3)
O(22)-P(1)-O(6)#6	110.8(7)	O(6)-Cs(5)-O(15)#11	78.6(3)
O(21)-P(1)-O(6)#6	105.8(7)	O(29)#11-Cs(5)-O(15)#11	91.3(3)
O(29)-P(1)-O(6)#6	101.8(8)	O(22)#12-Cs(5)-O(15)#11	132.3(3)
O(9)-P(2)-O(4)	108.8(7)	O(20)#8-Cs(5)-O(15)#11	134.8(4)
O(9)-P(2)-O(1)	111.9(7)	O(25)#7-Cs(5)-O(15)#11	92.2(3)
O(4)-P(2)-O(1)	110.1(6)	O(7)#7-Cs(5)-O(21)#12	128.0(3)
O(9)-P(2)-O(18)	113.4(7)	O(6)-Cs(5)-O(21)#12	94.1(3)
O(4)-P(2)-O(18)	109.3(6)	O(29)#11-Cs(5)-O(21)#12	49.2(3)
O(1)-P(2)-O(18)	103.2(6)	O(22)#12-Cs(5)-O(21)#12	45.0(3)
O(15)-P(3)-O(23)	113.9(8)	O(20)#8-Cs(5)-O(21)#12	119.5(4)
O(15)-P(3)-O(5)	113.5(7)	O(25)#7-Cs(5)-O(21)#12	172.5(3)
O(23)-P(3)-O(5)	111.3(7)	O(15)#11-Cs(5)-O(21)#12	90.0(3)
O(15)-P(3)-O(6)	108.1(7)	O(7)#7-Cs(5)-O(11)#7	43.9(3)
O(23)-P(3)-O(6)	104.9(7)	O(6)-Cs(5)-O(11)#7	176.8(3)
O(5)-P(3)-O(6)	104.2(7)	O(29)#11-Cs(5)-O(11)#7	134.4(3)
O(19)-P(4)-O(12)	115.3(8)	O(22)#12-Cs(5)-O(11)#7	66.1(3)
O(19)-P(4)-O(25)	114.2(8)	O(20)#8-Cs(5)-O(11)#7	110.1(4)
O(12)-P(4)-O(25)	111.2(8)	O(25)#7-Cs(5)-O(11)#7	85.0(3)
O(19)-P(4)-O(7)	106.6(7)	O(15)#11-Cs(5)-O(11)#7	104.1(3)
O(12)-P(4)-O(7)	107.1(7)	O(21)#12-Cs(5)-O(11)#7	87.5(3)
O(25)-P(4)-O(7)	101.0(7)	O(7)#7-Cs(5)-O(23)	94.1(3)
O(27)-P(5)-O(20)	117.7(9)	O(6)-Cs(5)-O(23)	42.0(3)
O(27)-P(5)-O(28)	111.5(9)	O(29)#11-Cs(5)-O(23)	88.1(3)
O(20)-P(5)-O(28)	105.4(9)	O(22)#12-Cs(5)-O(23)	141.4(3)
O(27)-P(5)-O(13)	105.9(8)	O(20)#8-Cs(5)-O(23)	55.8(4)
O(20)-P(5)-O(13)	108.9(8)	O(25)#7-Cs(5)-O(23)	51.5(3)
O(28)-P(5)-O(13)	107.1(9)	O(15)#11-Cs(5)-O(23)	79.1(3)
O(26)-P(6)-O(24)	115.3(9)	O(21)#12-Cs(5)-O(23)	136.0(3)
O(26)-P(6)-O(16)	114.6(9)	O(11)#7-Cs(5)-O(23)	136.5(3)
O(24)-P(6)-O(16)	110.6(8)	O(11)-P(7)-O(17)	113.3(8)
O(26)-P(6)-O(13)	107.7(8)	O(11)-P(7)-O(8)	112.1(7)
O(24)-P(6)-O(13)	106.6(8)	O(17)-P(7)-O(8)	112.4(7)
O(16)-P(6)-O(13)	100.7(8)	O(11)-P(7)-O(7)	104.4(7)
O(10)-P(8)-O(2)	110.7(7)	O(17)-P(7)-O(7)	106.3(7)

O(10)-P(8)-O(14)	110.0(7)	O(8)-P(7)-O(7)	107.6(7)
O(2)-P(8)-O(14)	111.2(7)	O(2)-P(8)-O(3)	104.6(6)
O(10)-P(8)-O(3)	110.8(7)	O(14)-P(8)-O(3)	109.4(7)

Symmetry transformations used to generate equivalent atoms:

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

#3 -x+2, y+1/2, -z+3/2 #4 x+1, y, z #5 -x+2, -y+1, -z+2

#6 -x+1, y-1/2, -z+3/2 #7 x, y+1, z #8 x-1, y, z

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

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

#13 x+1, y-1, z #14 x, y-1, z #15 -x+2, y-1/2, -z+3/2

Table S7. Bond lengths (Å) and angles (°) for $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$.

Bi(1)-O(7)	2.174(10)	Cs(1)-O(10)	3.083(11)
Bi(1)-O(2)#1	2.252(10)	Cs(1)-O(27)	3.112(15)
Bi(1)-O(24)#2	2.319(11)	Cs(1)-O(19)	3.188(11)
Bi(1)-O(19)	2.368(11)	Cs(1)-O(13)	3.197(11)
Bi(1)-O(15)#2	2.449(12)	Cs(1)-O(14)#11	3.247(11)
Bi(1)-O(26)#3	2.665(13)	Cs(1)-O(18)	3.309(11)
Bi(2)-O(1)	2.145(10)	Cs(1)-O(24)	3.329(11)
Bi(2)-O(4)#4	2.186(11)	Cs(1)-O(14)	3.356(11)
Bi(2)-O(11)#5	2.252(10)	Cs(2)-O(8)#5	2.904(10)
Bi(2)-O(17)	2.521(11)	Cs(2)-O(28)#2	2.995(13)
Bi(2)-O(28)#2	2.722(12)	Cs(2)-O(6)#2	3.075(10)
Bi(2)-O(5)#2	2.725(11)	Cs(2)-O(13)#2	3.139(10)
Bi(3)-O(12)#7	2.169(11)	Cs(2)-O(23)#2	3.214(13)
Bi(3)-O(3)	2.192(9)	Cs(2)-O(3)#5	3.218(10)
Bi(3)-O(8)	2.201(10)	Cs(2)-O(3)	3.360(10)
Bi(3)-O(21)#2	2.573(12)	Cs(2)-O(9)	3.389(10)
Bi(3)-O(5)#2	2.631(11)	Cs(2)-O(11)#5	3.505(11)
Bi(3)-O(23)	2.671(12)	Cs(2)-O(11)	3.543(11)
Bi(4)-O(20)	2.192(11)	Cs(2)-O(5)#2	3.624(10)
Bi(4)-O(25)#3	2.213(13)	Cs(4)-O(1)#6	3.052(10)
Bi(4)-O(9)#8	2.250(10)	Cs(4)-O(28)#2	3.079(12)
Bi(4)-O(13)	2.420(11)	Cs(4)-O(22)#12	3.118(11)
Bi(4)-O(29)	2.487(12)	Cs(4)-O(4)#5	3.128(11)
Bi(4)-O(21)	2.538(11)	Cs(4)-O(9)#4	3.283(9)
Cs(3)-O(6)	2.933(11)	Cs(4)-O(12)#6	3.316(10)
Cs(3)-O(27)	2.979(13)	Cs(4)-O(1)#2	3.334(9)
Cs(3)-O(16)	3.001(11)	Cs(4)-O(6)#2	3.374(11)
Cs(3)-O(17)	3.024(11)	Cs(4)-O(17)#2	3.568(11)
Cs(3)-O(15)#2	3.093(11)	Cs(5)-O(16)#3	3.088(11)
Cs(3)-O(23)	3.237(13)	Cs(5)-O(27)#3	3.087(14)
Cs(3)-O(5)#2	3.385(10)	Cs(5)-O(24)#10	3.175(11)
P(1)-O(26)	1.489(13)	Cs(5)-O(19)	3.252(12)
P(1)-O(17)	1.499(12)	Cs(5)-O(29)	3.267(12)
P(1)-O(21)#12	1.531(12)	Cs(5)-O(2)#1	3.288(10)
P(1)-O(22)#4	1.619(11)	Cs(5)-O(14)#10	3.471(11)
P(2)-O(6)	1.508(11)	Cs(5)-O(20)	3.501(12)
P(2)-O(8)	1.542(10)	Cs(5)-O(14)	3.553(11)
P(2)-O(12)	1.552(11)	Cs(5)-O(22)	3.715(10)
P(2)-O(1)	1.567(10)	Cs(5)-O(26)#3	3.720(13)
P(3)-O(13)	1.499(11)	Cs(6)-O(18)#10	2.995(10)
P(3)-O(15)	1.510(11)	Cs(6)-O(10)	3.019(11)
P(3)-O(5)	1.522(11)	Cs(6)-O(26)#1	3.108(13)
P(3)-O(18)	1.613(11)	Cs(6)-O(16)#1	3.142(11)

P(4)-O(14)	1.486(11)	Cs(6)-O(7)	3.281(10)
P(4)-O(29)	1.512(12)	Cs(6)-O(25)#10	3.349(12)
P(4)-O(24)	1.526(12)	Cs(6)-O(14)	3.350(11)
P(4)-O(10)#10	1.626(11)	Cs(6)-O(2)#1	3.379(9)
P(5)-O(16)	1.480(12)	Cs(6)-O(29)#11	3.461(12)
P(5)-O(2)	1.534(10)	Cs(6)-O(15)#10	3.567(12)
P(5)-O(7)	1.545(11)	P(7)-O(11)	1.522(10)
P(5)-O(10)	1.636(10)	P(7)-O(4)	1.537(11)
P(6)-O(23)	1.460(13)	P(7)-O(3)	1.540(10)
P(6)-O(20)	1.520(11)	P(7)-O(9)	1.564(10)
P(6)-O(19)	1.531(12)	P(8)-O(27)	1.450(14)
P(6)-O(22)	1.618(11)	P(8)-O(28)	1.498(12)
O(7)-Bi(1)-O(2)#1	80.0(4)	P(8)-O(25)	1.527(13)
O(7)-Bi(1)-O(24)#2	90.3(4)	P(8)-O(18)	1.637(11)
O(2)#1-Bi(1)-O(24)#2	83.0(4)		
O(7)-Bi(1)-O(19)	83.8(4)	O(1)-Bi(2)-O(4)#4	83.1(4)
O(2)#1-Bi(1)-O(19)	91.4(4)	O(1)-Bi(2)-O(11)#5	86.4(4)
O(24)#2-Bi(1)-O(19)	172.6(4)	O(4)#4-Bi(2)-O(11)#5	85.0(4)
O(7)-Bi(1)-O(15)#2	92.4(4)	O(1)-Bi(2)-O(17)	80.5(4)
O(2)#1-Bi(1)-O(15)#2	165.6(4)	O(4)#4-Bi(2)-O(17)	91.6(4)
O(24)#2-Bi(1)-O(15)#2	84.8(4)	O(11)#5-Bi(2)-O(17)	166.7(4)
O(19)-Bi(1)-O(15)#2	99.9(4)	O(1)-Bi(2)-O(28)#2	158.4(4)
O(7)-Bi(1)-O(26)#3	149.5(4)	O(4)#4-Bi(2)-O(28)#2	113.4(4)
O(2)#1-Bi(1)-O(26)#3	77.2(4)	O(11)#5-Bi(2)-O(28)#2	81.5(4)
O(24)#2-Bi(1)-O(26)#3	106.6(4)	O(17)-Bi(2)-O(28)#2	111.6(4)
O(19)-Bi(1)-O(26)#3	76.9(4)	O(1)-Bi(2)-O(5)#2	90.7(3)
O(15)#2-Bi(1)-O(26)#3	113.8(4)	O(4)#4-Bi(2)-O(5)#2	173.6(3)
O(12)#7-Bi(3)-O(3)	88.5(4)	O(11)#5-Bi(2)-O(5)#2	96.0(3)
O(12)#7-Bi(3)-O(8)	89.9(4)	O(17)-Bi(2)-O(5)#2	85.9(3)
O(3)-Bi(3)-O(8)	81.5(4)	O(28)#2-Bi(2)-O(5)#2	73.0(3)
O(12)#7-Bi(3)-O(21)#2	98.0(4)	O(20)-Bi(4)-O(25)#3	96.5(4)
O(3)-Bi(3)-O(21)#2	77.8(4)	O(20)-Bi(4)-O(9)#8	83.0(4)
O(8)-Bi(3)-O(21)#2	157.5(3)	O(25)#3-Bi(4)-O(9)#8	86.7(4)
O(12)#7-Bi(3)-O(5)#2	168.7(4)	O(20)-Bi(4)-O(13)	87.3(4)
O(3)-Bi(3)-O(5)#2	87.4(3)	O(25)#3-Bi(4)-O(13)	176.2(4)
O(8)-Bi(3)-O(5)#2	79.0(3)	O(9)#8-Bi(4)-O(13)	94.1(4)
O(21)#2-Bi(3)-O(5)#2	91.4(3)	O(20)-Bi(4)-O(29)	84.8(4)
O(12)#7-Bi(3)-O(23)	84.7(4)	O(25)#3-Bi(4)-O(29)	83.5(4)
O(3)-Bi(3)-O(23)	154.6(4)	O(9)#8-Bi(4)-O(29)	163.3(4)
O(8)-Bi(3)-O(23)	122.9(4)	O(13)-Bi(4)-O(29)	96.5(4)
O(21)#2-Bi(3)-O(23)	79.0(4)	O(20)-Bi(4)-O(21)	161.0(4)
O(5)#2-Bi(3)-O(23)	103.3(4)	O(25)#3-Bi(4)-O(21)	93.5(4)
O(10)-Cs(1)-O(27)	96.6(3)	O(9)#8-Bi(4)-O(21)	81.4(4)
O(10)-Cs(1)-O(19)	92.1(3)	O(13)-Bi(4)-O(21)	83.0(4)

O(27)-Cs(1)-O(19)	110.4(3)	O(29)-Bi(4)-O(21)	112.5(4)
O(10)-Cs(1)-O(13)	174.7(3)	O(8)#5-Cs(2)-O(28)#2	133.6(3)
O(27)-Cs(1)-O(13)	78.5(3)	O(8)#5-Cs(2)-O(6)#2	66.7(3)
O(19)-Cs(1)-O(13)	91.8(3)	O(28)#2-Cs(2)-O(6)#2	77.2(3)
O(10)-Cs(1)-O(14)#11	46.6(3)	O(8)#5-Cs(2)-O(13)#2	152.4(3)
O(27)-Cs(1)-O(14)#11	76.0(3)	O(28)#2-Cs(2)-O(13)#2	72.4(3)
O(19)-Cs(1)-O(14)#11	138.4(3)	O(6)#2-Cs(2)-O(13)#2	121.9(3)
O(13)-Cs(1)-O(14)#11	129.1(3)	O(8)#5-Cs(2)-O(23)#2	84.8(3)
O(10)-Cs(1)-O(18)	130.0(3)	O(28)#2-Cs(2)-O(23)#2	101.5(3)
O(27)-Cs(1)-O(18)	44.6(3)	O(6)#2-Cs(2)-O(23)#2	59.3(3)
O(19)-Cs(1)-O(18)	126.6(3)	O(13)#2-Cs(2)-O(23)#2	79.8(3)
O(13)-Cs(1)-O(18)	44.7(3)	O(8)#5-Cs(2)-O(3)#5	55.6(3)
O(14)#11-Cs(1)-O(18)	87.8(3)	O(28)#2-Cs(2)-O(3)#5	91.0(3)
O(10)-Cs(1)-O(24)	107.4(3)	O(6)#2-Cs(2)-O(3)#5	79.9(3)
O(27)-Cs(1)-O(24)	125.7(3)	O(13)#2-Cs(2)-O(3)#5	146.9(3)
O(19)-Cs(1)-O(24)	116.4(3)	O(23)#2-Cs(2)-O(3)#5	132.6(3)
O(13)-Cs(1)-O(24)	74.1(3)	O(8)#5-Cs(2)-O(3)	100.0(3)
O(14)#11-Cs(1)-O(24)	86.3(3)	O(28)#2-Cs(2)-O(3)	113.2(3)
O(18)-Cs(1)-O(24)	84.5(3)	O(6)#2-Cs(2)-O(3)	166.6(3)
O(10)-Cs(1)-O(14)	79.0(3)	O(13)#2-Cs(2)-O(3)	70.7(3)
O(27)-Cs(1)-O(14)	164.5(3)	O(23)#2-Cs(2)-O(3)	123.5(3)
O(19)-Cs(1)-O(14)	84.8(3)	O(3)#5-Cs(2)-O(3)	91.1(2)
O(13)-Cs(1)-O(14)	105.1(3)	O(8)#5-Cs(2)-O(9)	91.7(3)
O(14)#11-Cs(1)-O(14)	90.52(3)	O(28)#2-Cs(2)-O(9)	134.7(3)
O(18)-Cs(1)-O(14)	128.6(3)	O(6)#2-Cs(2)-O(9)	133.9(3)
O(24)-Cs(1)-O(14)	44.1(3)	O(13)#2-Cs(2)-O(9)	63.1(3)
O(6)-Cs(3)-O(27)	104.3(3)	O(23)#2-Cs(2)-O(9)	79.3(3)
O(6)-Cs(3)-O(16)	176.2(3)	O(3)#5-Cs(2)-O(9)	122.0(2)
O(27)-Cs(3)-O(16)	75.6(3)	O(3)-Cs(2)-O(9)	44.5(2)
O(6)-Cs(3)-O(17)	82.3(3)	O(8)#5-Cs(2)-O(11)#5	98.4(3)
O(27)-Cs(3)-O(17)	108.2(3)	O(28)#2-Cs(2)-O(11)#5	59.7(3)
O(16)-Cs(3)-O(17)	101.3(3)	O(6)#2-Cs(2)-O(11)#5	100.4(3)
O(6)-Cs(3)-O(15)#2	107.2(3)	O(13)#2-Cs(2)-O(11)#5	105.0(3)
O(27)-Cs(3)-O(15)#2	143.5(3)	O(23)#2-Cs(2)-O(11)#5	156.5(3)
O(16)-Cs(3)-O(15)#2	71.8(3)	O(3)#5-Cs(2)-O(11)#5	43.0(2)
O(17)-Cs(3)-O(15)#2	94.0(3)	O(3)-Cs(2)-O(11)#5	79.1(2)
O(6)-Cs(3)-O(23)	60.4(3)	O(9)-Cs(2)-O(11)#5	123.6(2)
O(27)-Cs(3)-O(23)	101.8(4)	O(8)#5-Cs(2)-O(11)	60.5(3)
O(16)-Cs(3)-O(23)	115.9(3)	O(28)#2-Cs(2)-O(11)	152.7(3)
O(17)-Cs(3)-O(23)	136.8(3)	O(6)#2-Cs(2)-O(11)	125.8(3)
O(15)#2-Cs(3)-O(23)	78.6(3)	O(13)#2-Cs(2)-O(11)	101.0(3)
O(6)-Cs(3)-O(5)#2	67.3(3)	O(23)#2-Cs(2)-O(11)	103.3(3)
O(27)-Cs(3)-O(5)#2	170.7(3)	O(3)#5-Cs(2)-O(11)	80.5(2)
O(16)-Cs(3)-O(5)#2	113.0(3)	O(3)-Cs(2)-O(11)	42.0(2)

O(17)-Cs(3)-O(5)#2	67.6(3)	O(9)-Cs(2)-O(11)	42.0(2)
O(15)#2-Cs(3)-O(5)#2	45.7(3)	O(11)#5-Cs(2)-O(11)	98.4(2)
O(23)-Cs(3)-O(5)#2	77.8(3)	O(8)#5-Cs(2)-O(5)#2	151.3(3)
O(16)#3-Cs(5)-O(27)#3	72.8(3)	O(28)#2-Cs(2)-O(5)#2	57.7(3)
O(16)#3-Cs(5)-O(24)#10	63.9(3)	O(6)#2-Cs(2)-O(5)#2	134.6(3)
O(27)#3-Cs(5)-O(24)#10	110.6(3)	O(13)#2-Cs(2)-O(5)#2	42.9(3)
O(16)#3-Cs(5)-O(19)	124.0(3)	O(23)#2-Cs(2)-O(5)#2	121.5(3)
O(27)#3-Cs(5)-O(19)	111.0(3)	O(3)#5-Cs(2)-O(5)#2	104.0(2)
O(24)#10-Cs(5)-O(19)	137.8(3)	O(3)-Cs(2)-O(5)#2	57.2(2)
O(16)#3-Cs(5)-O(29)	149.1(3)	O(9)-Cs(2)-O(5)#2	82.9(2)
O(27)#3-Cs(5)-O(29)	80.7(3)	O(11)#5-Cs(2)-O(5)#2	62.7(2)
O(24)#10-Cs(5)-O(29)	113.3(3)	O(11)-Cs(2)-O(5)#2	99.1(2)
O(19)-Cs(5)-O(29)	80.0(3)	O(1)#6-Cs(4)-O(28)#2	135.6(3)
O(16)#3-Cs(5)-O(2)#1	87.9(3)	O(1)#6-Cs(4)-O(22)#12	114.6(3)
O(27)#3-Cs(5)-O(2)#1	149.6(3)	O(28)#2-Cs(4)-O(22)#12	103.4(3)
O(24)#10-Cs(5)-O(2)#1	79.7(3)	O(1)#6-Cs(4)-O(4)#5	55.4(3)
O(19)-Cs(5)-O(2)#1	60.8(3)	O(28)#2-Cs(4)-O(4)#5	82.6(3)
O(29)-Cs(5)-O(2)#1	122.6(3)	O(22)#12-Cs(4)-O(4)#5	165.4(3)
O(16)#3-Cs(5)-O(14)#10	72.2(3)	O(1)#6-Cs(4)-O(9)#4	87.5(2)
O(27)#3-Cs(5)-O(14)#10	73.1(3)	O(28)#2-Cs(4)-O(9)#4	70.4(3)
O(24)#10-Cs(5)-O(14)#10	44.1(3)	O(22)#12-Cs(4)-O(9)#4	89.1(3)
O(19)-Cs(5)-O(14)#10	163.7(3)	O(4)#5-Cs(4)-O(9)#4	80.3(3)
O(29)-Cs(5)-O(14)#10	85.3(3)	O(1)#6-Cs(4)-O(12)#6	45.1(3)
O(2)#1-Cs(5)-O(14)#10	123.8(3)	O(28)#2-Cs(4)-O(12)#6	164.6(3)
O(16)#3-Cs(5)-O(20)	126.5(3)	O(22)#12-Cs(4)-O(12)#6	70.3(3)
O(27)#3-Cs(5)-O(20)	71.7(3)	O(4)#5-Cs(4)-O(12)#6	100.5(3)
O(24)#10-Cs(5)-O(20)	168.6(3)	O(9)#4-Cs(4)-O(12)#6	95.1(2)
O(19)-Cs(5)-O(20)	43.4(3)	O(1)#6-Cs(4)-O(1)#2	85.1(3)
O(29)-Cs(5)-O(20)	55.6(3)	O(28)#2-Cs(4)-O(1)#2	116.1(3)
O(2)#1-Cs(5)-O(20)	103.9(3)	O(22)#12-Cs(4)-O(1)#2	92.8(3)
O(14)#10-Cs(5)-O(20)	130.4(3)	O(4)#5-Cs(4)-O(1)#2	96.4(2)
O(16)#3-Cs(5)-O(14)	147.6(3)	O(9)#4-Cs(4)-O(1)#2	172.5(2)
O(27)#3-Cs(5)-O(14)	121.1(3)	O(12)#6-Cs(4)-O(1)#2	78.8(2)
O(24)#10-Cs(5)-O(14)	83.7(3)	O(1)#6-Cs(4)-O(6)#2	116.0(3)
O(19)-Cs(5)-O(14)	80.8(3)	O(28)#2-Cs(4)-O(6)#2	71.7(3)
O(29)-Cs(5)-O(14)	43.4(3)	O(22)#12-Cs(4)-O(6)#2	105.8(3)
O(2)#1-Cs(5)-O(14)	87.7(2)	O(4)#5-Cs(4)-O(6)#2	88.6(3)
O(14)#10-Cs(5)-O(14)	83.77(3)	O(9)#4-Cs(4)-O(6)#2	141.5(2)
O(20)-Cs(5)-O(14)	85.7(3)	O(12)#6-Cs(4)-O(6)#2	123.2(2)
O(16)#3-Cs(5)-O(22)	93.5(3)	O(1)#2-Cs(4)-O(6)#2	44.5(2)
O(27)#3-Cs(5)-O(22)	74.9(3)	O(1)#6-Cs(4)-O(17)#2	114.3(2)
O(24)#10-Cs(5)-O(22)	152.0(3)	O(28)#2-Cs(4)-O(17)#2	109.1(3)
O(19)-Cs(5)-O(22)	42.0(3)	O(22)#12-Cs(4)-O(17)#2	42.4(3)
O(29)-Cs(5)-O(22)	94.6(3)	O(4)#5-Cs(4)-O(17)#2	148.3(3)

O(2)#1-Cs(5)-O(22)	83.3(2)	O(9)#4-Cs(4)-O(17)#2	131.2(2)
O(14)#10-Cs(5)-O(22)	147.6(3)	O(12)#6-Cs(4)-O(17)#2	76.2(3)
O(20)-Cs(5)-O(22)	39.0(2)	O(1)#2-Cs(4)-O(17)#2	51.9(2)
O(14)-Cs(5)-O(22)	117.8(2)	O(6)#2-Cs(4)-O(17)#2	68.7(3)
O(16)#3-Cs(5)-O(26)#3	71.1(3)	O(17)#2-Cs(4)-O(20)#12	81.7(2)
O(27)#3-Cs(5)-O(26)#3	99.0(3)	O(18)#10-Cs(6)-O(10)	140.0(3)
O(24)#10-Cs(5)-O(26)#3	113.5(3)	O(18)#10-Cs(6)-O(26)#1	92.8(3)
O(19)-Cs(5)-O(26)#3	53.0(3)	O(10)-Cs(6)-O(26)#1	74.8(3)
O(29)-Cs(5)-O(26)#3	129.8(3)	O(18)#10-Cs(6)-O(16)#1	102.7(3)
O(2)#1-Cs(5)-O(26)#3	51.8(3)	O(10)-Cs(6)-O(16)#1	111.8(3)
O(14)#10-Cs(5)-O(26)#3	143.2(3)	O(26)#1-Cs(6)-O(16)#1	79.3(3)
O(20)-Cs(5)-O(26)#3	76.4(3)	O(18)#10-Cs(6)-O(7)	174.8(3)
O(14)-Cs(5)-O(26)#3	128.0(3)	O(10)-Cs(6)-O(7)	45.2(3)
O(22)-Cs(5)-O(26)#3	39.6(3)	O(26)#1-Cs(6)-O(7)	88.5(3)
O(26)-P(1)-O(17)	117.4(7)	O(16)#1-Cs(6)-O(7)	72.6(3)
O(26)-P(1)-O(21)#12	108.4(7)	O(18)#10-Cs(6)-O(25)#10	44.4(3)
O(17)-P(1)-O(21)#12	112.6(7)	O(10)-Cs(6)-O(25)#10	98.6(3)
O(26)-P(1)-O(22)#4	108.2(7)	O(26)#1-Cs(6)-O(25)#10	60.7(3)
O(17)-P(1)-O(22)#4	103.7(6)	O(16)#1-Cs(6)-O(25)#10	120.7(3)
O(21)#12-P(1)-O(22)#4	105.7(6)	O(7)-Cs(6)-O(25)#10	139.8(3)
O(6)-P(2)-O(8)	107.5(6)	O(18)#10-Cs(6)-O(14)	91.3(3)
O(6)-P(2)-O(12)	115.1(6)	O(10)-Cs(6)-O(14)	79.9(3)
O(8)-P(2)-O(12)	110.2(6)	O(26)#1-Cs(6)-O(14)	145.2(3)
O(6)-P(2)-O(1)	111.2(6)	O(16)#1-Cs(6)-O(14)	133.1(3)
O(8)-P(2)-O(1)	108.9(6)	O(7)-Cs(6)-O(14)	90.5(3)
O(12)-P(2)-O(1)	103.8(6)	O(25)#10-Cs(6)-O(14)	100.6(3)
O(13)-P(3)-O(15)	113.7(6)	O(18)#10-Cs(6)-O(2)#1	124.6(3)
O(13)-P(3)-O(5)	112.7(6)	O(10)-Cs(6)-O(2)#1	94.6(3)
O(15)-P(3)-O(5)	113.2(6)	O(26)#1-Cs(6)-O(2)#1	115.7(3)
O(13)-P(3)-O(18)	105.4(6)	O(16)#1-Cs(6)-O(2)#1	45.7(3)
O(15)-P(3)-O(18)	103.1(6)	O(7)-Cs(6)-O(2)#1	50.6(3)
O(5)-P(3)-O(18)	107.7(6)	O(25)#10-Cs(6)-O(2)#1	164.5(3)
O(14)-P(4)-O(29)	115.4(6)	O(14)-Cs(6)-O(2)#1	89.6(2)
O(14)-P(4)-O(24)	113.1(7)	O(18)#10-Cs(6)-O(29)#11	96.3(3)
O(29)-P(4)-O(24)	111.5(7)	O(10)-Cs(6)-O(29)#11	44.2(3)
O(14)-P(4)-O(10)#10	107.3(6)	O(26)#1-Cs(6)-O(29)#11	61.0(3)
O(29)-P(4)-O(10)#10	103.9(6)	O(16)#1-Cs(6)-O(29)#11	136.7(3)
O(24)-P(4)-O(10)#10	104.5(6)	O(7)-Cs(6)-O(29)#11	88.7(3)
O(16)-P(5)-O(2)	115.1(6)	O(25)#10-Cs(6)-O(29)#11	54.8(3)
O(16)-P(5)-O(7)	114.3(6)	O(14)-Cs(6)-O(29)#11	84.2(3)
O(2)-P(5)-O(7)	109.7(6)	O(2)#1-Cs(6)-O(29)#11	138.8(3)
O(16)-P(5)-O(10)	110.4(6)	O(18)#10-Cs(6)-O(15)#10	42.7(3)
O(2)-P(5)-O(10)	106.1(6)	O(10)-Cs(6)-O(15)#10	175.3(3)
O(7)-P(5)-O(10)	99.8(6)	O(26)#1-Cs(6)-O(15)#10	101.9(3)

O(23)-P(6)-O(20)	115.0(7)	O(16)#1-Cs(6)-O(15)#10	64.0(3)
O(23)-P(6)-O(19)	114.3(7)	O(7)-Cs(6)-O(15)#10	132.1(3)
O(20)-P(6)-O(19)	110.4(6)	O(25)#10-Cs(6)-O(15)#10	82.5(3)
O(23)-P(6)-O(22)	108.1(7)	O(14)-Cs(6)-O(15)#10	104.4(3)
O(20)-P(6)-O(22)	100.8(6)	O(2)#1-Cs(6)-O(15)#10	83.8(2)
O(19)-P(6)-O(22)	107.1(6)	O(29)#11-Cs(6)-O(15)#10	137.2(3)
O(11)-P(7)-O(4)	110.5(6)	O(27)-P(8)-O(28)	119.1(7)
O(11)-P(7)-O(3)	108.0(6)	O(27)-P(8)-O(25)	113.5(8)
O(4)-P(7)-O(3)	109.3(6)	O(28)-P(8)-O(25)	108.7(7)
O(11)-P(7)-O(9)	107.5(6)	O(27)-P(8)-O(18)	104.6(7)
O(4)-P(7)-O(9)	110.8(6)	O(28)-P(8)-O(18)	109.3(6)
O(3)-P(7)-O(9)	110.8(6)	O(25)-P(8)-O(18)	99.8(6)

Symmetry transformations used to generate equivalent atoms:

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

Table S8. Some reported bismuth phosphates containing alkali metals or alkaline earth metals cations.

Compounds	Space Group	Dimension	Reference
$Li_2KBi(PO_4)_2$	$P2_1$	1D	1
$Li_2RbBi(PO_4)_2$	$C2$	1D	1
$Li_2CsBi(PO_4)_2$	$C2$	1D	1
$K_3SrBi(P_2O_7)_2$	$P2_1$	2D	2
$Rb_3SrBi(P_2O_7)_2$	$P2_1$	2D	2
$Rb_3PbBi(P_2O_7)_2$	$P2_1$	2D	3
$Cs_3PbBi(P_2O_7)_2$	$P2_12_12_1$	2D	3
$Rb_3BaBi(P_2O_7)_2$	$P2_1$	2D	4
$Cs_3BaBi(P_2O_7)_2$	$P2_12_12_1$	2D	4
$Cs_3SrBi(P_2O_7)_2$	$P2_12_12_1$	2D	5
$Cs_3CaBi(P_2O_7)_2$	$P2_12_12_1$	2D	5
$Rb_2PbBi_2(PO_4)_2(P_2O_7)$	$Pnma$	3D	6
$Cs_2PbBi_2(PO_4)_2(P_2O_7)$	$Pnma$	3D	6
$Rb_6Bi_4(PO_4)_2(P_2O_7)_3$	$P2_1/c$	3D	7
$\mathbf{Cs_6Bi_4(PO_4)_2(P_2O_7)_3}$	$\boldsymbol{P2_1/c}$	**3D**	**The Article**
$\mathbf{RbCs_5Bi_4(PO_4)_2(P_2O_7)_3}$	$\boldsymbol{P2_1/c}$	**3D**	**The Article**
$\mathbf{KCs_5Bi_4(PO_4)_2(P_2O_7)_3}$	$\boldsymbol{P2_1/c}$	**3D**	**The Article**

Table S9. Some reported phosphates designed by dimensional reduction theory.

Compounds	Parents [a]	Dimensional reduction agents [a]	Equivalent
$Cs_2PbBi_2(PO_4)_2(P_2O_7)$[6]	$CsBiP_2O_7$	PbO	1/2
$Rb_2PbBi_2(PO_4)_2(P_2O_7)$[6]	$Bi_2P_4O_{13}$	PbO, Rb_2O	1, 1
$Pb_9[Li_2(P_2O_7)_2(P_4O_{13})_2]$[8]	$Pb_3P_4O_{13}$	Li_2O	1/3
$Pb_{12}[Li_2(P_2O_7)_2(P_4O_{13})_2](P_4O_{13})$[9]	$Pb_3P_4O_{13}$	Li_2O	1/4
$Rb_6Bi_4(PO_4)_2(P_2O_7)_3$[7]	$Bi_2P_4O_{13}$	Rb_2O	3/2
$Cs_6Bi_4(PO_4)_2(P_2O_7)_3$	$CsBiP_2O_7$	Cs_2O	1/4
$RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$	$CsBiP_2O_7$	Cs_2O, Rb_2O	1/8, 1/8
$KCs_5Bi_4(PO_4)_2(P_2O_7)_3$	$CsBiP_2O_7$	Cs_2O, K_2O	1/8, 1/8
$Th_4(PO_4)_4(P_2O_7)$[10]	ThP_2O_7	ThO_2	1/3
$U_2(PO_4)(P_3O_{10})$[11]	$U(PO_3)_4$	UO_2	1
$Na_4Ni_5(PO_4)_2(P_2O_7)_2$[12]	$NaNi(PO_3)_3$	Na_2O, NiO	1/2, 3/2
$Na_4A_3(PO_4)_2(P_2O_7)$ (A = Mg, Mn, Fe, Co and Ni)[13,14]	$A_2P_4O_{12}$	Na_2O, AO	2, 1
$Ni_4M_2(PO_4)_2(P_2O_7)$ (M = K, Tl)[15]	$Ni_2P_2O_7$	M_2O	1/2
$Li_9Al_3(PO_4)_2(P_2O_7)_3$[16]	$LiAl(PO_3)_4$	Li_2O, Al_2O_3	7/2, 1/4
$LiMg_3(PO_4)(P_2O_7)$[17]	$Mg_2P_2O_7$	Li_2O	1/3
$KNi_3(PO_4)(P_2O_7)$[18]	$Ni_2P_2O_7$	K_2O	1/3
$Eu_2Si(PO_4)_2(P_2O_7)$[19]	EuP_5O_{14}	Eu_2O_3, SiO_2	3/5, 1
$MnSr_2(PO_4)(P_2O_7)$[20]	$Sr(PO_3)_2$	Mn_2O_3, SrO	1/2, 1/3
$VCa_2(PO_4)(P_2O_7)$[21]	$Ca(PO_3)_2$	V_2O_3, CaO	1/2, 1/3
$MoPb_2(PO_4)(P_2O_7)$[22]	$Pb(PO_3)_2$	Mo_2O_3, PbO	1/2, 1/3
$AgN_2(PO_4)(P_2O_7)$ (N = V, Cr)[23]	$N(PO_3)_3$	N_2O_3, Ag_2O	1/2, 1/2
$KX_6(P_2O_7)_2(P_3O_{10})$ (M = Cd, Mg)[24,25]	$X(PO_3)_2$	XO, K_2O	5/7, 1/2
$AMn_6(P_2O_7)_2(P_3O_{10})$ (A = Na, Ag, K)[25,26]	$Mn(PO_3)_2$	MnO, A_2O	5/7, 1/2
$Na_7Y_2(P_2O_7)_2(P_3O_{10})$[27]	$NaPO_3$	Y_2O_3	1/7

[a] A compounds can possess different parents when different agents are selected as dimensional reduction agents. For example, in $Cs_2PbBi_2(PO_4)_2(P_2O_7)$, when selecting PbO as dimensional reduction agent, $CsBiP_2O_7$ is regard as parent; when selecting Cs_2O and PbO as dimensional reduction agent, $Bi_2P_4O_{13}$ is regard as parent.

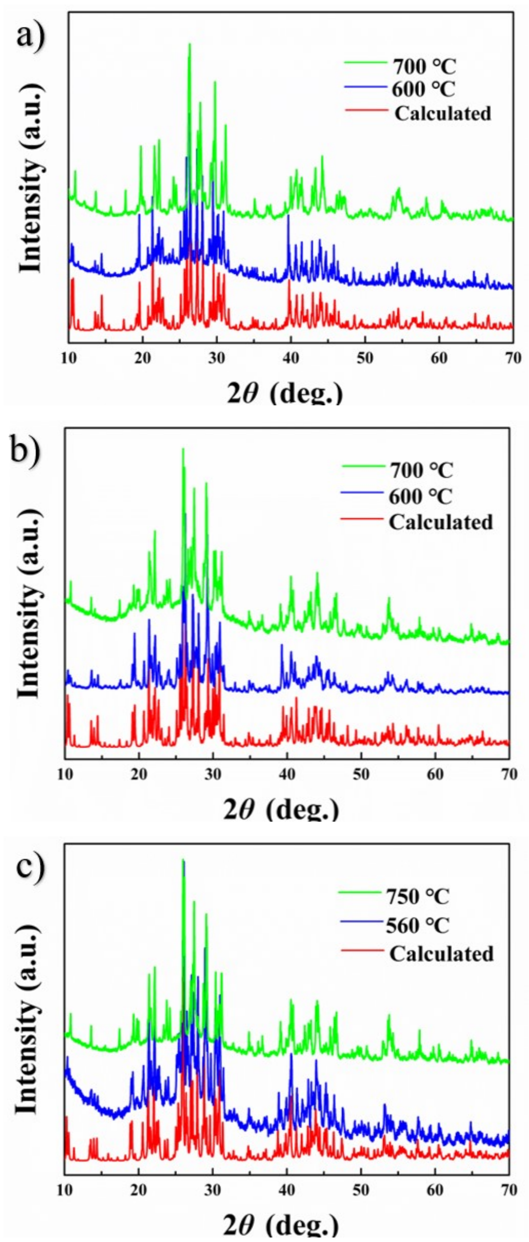

Figure S1. PXRD spectra of a) $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$, b) $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$ and c) $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$.

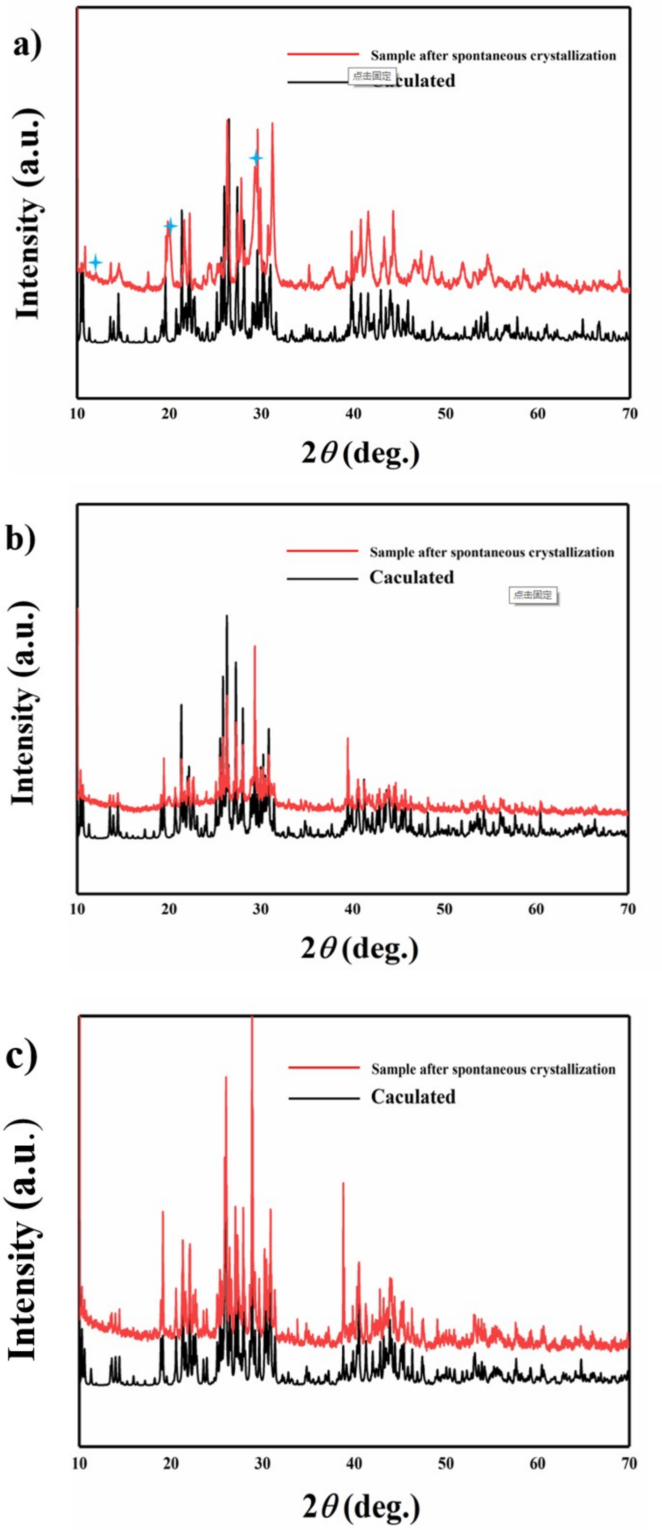

Figure S2. PXRD of a) $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$, b) $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$ and c) $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$ after spontaneous crystallization

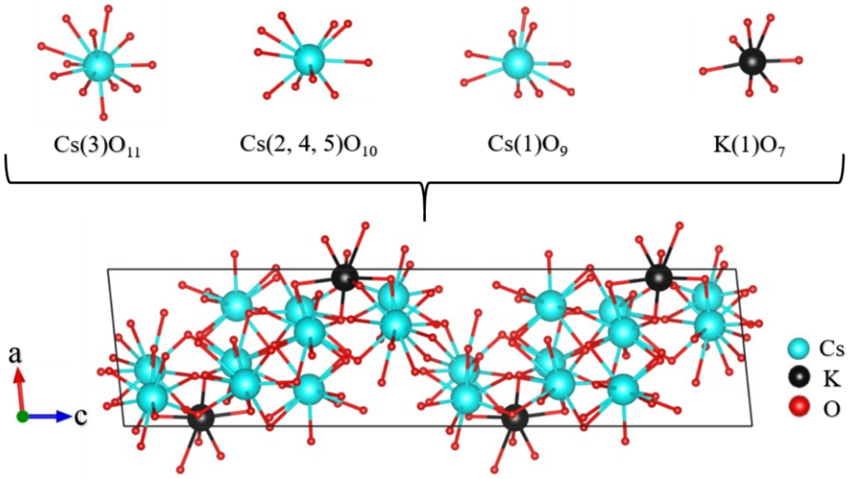

Figure S3. Coordination environment of K^+ and Cs^+ cations in $KCs_5Bi_4(P_2O_7)_3(PO_4)_2$.

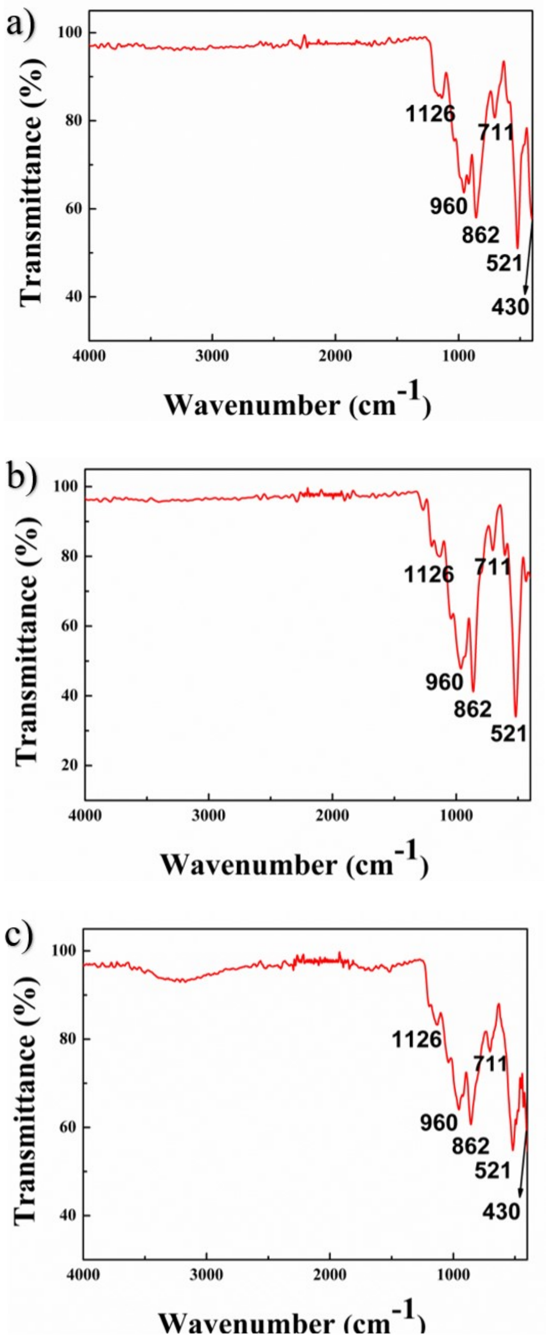

Figure S4. IR spectra of a) $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$, b) $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$ and c) $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$.

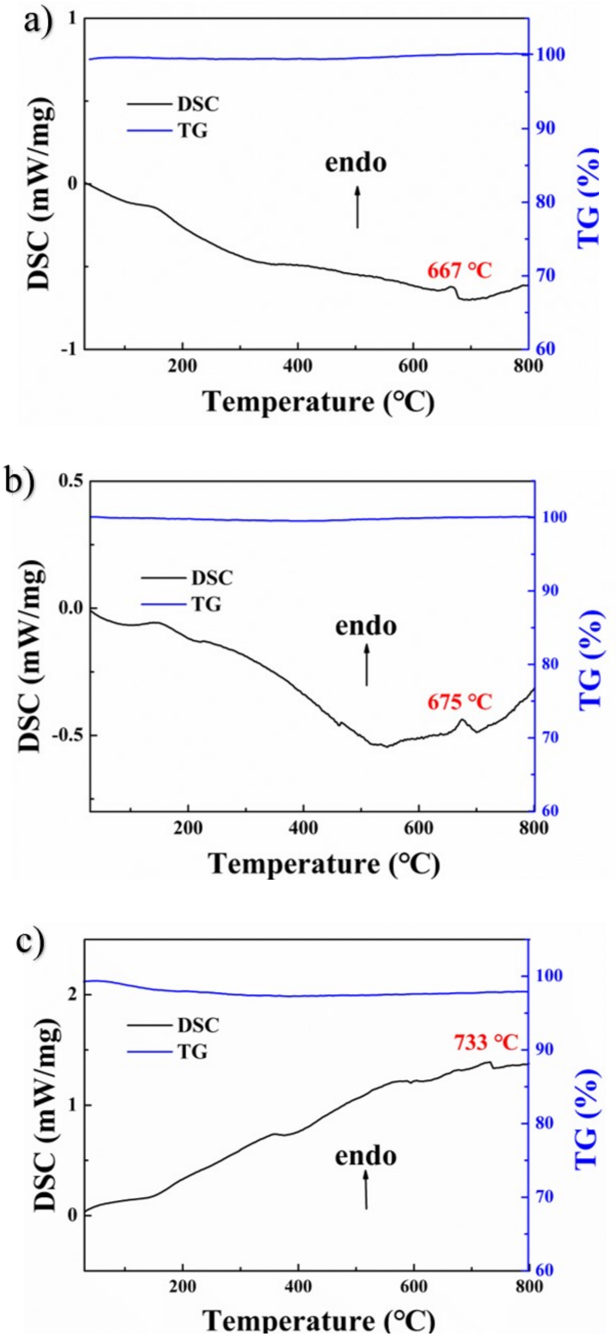

Figure S5. TG and DSC curves of a) $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$, b) $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$ and c) $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$.

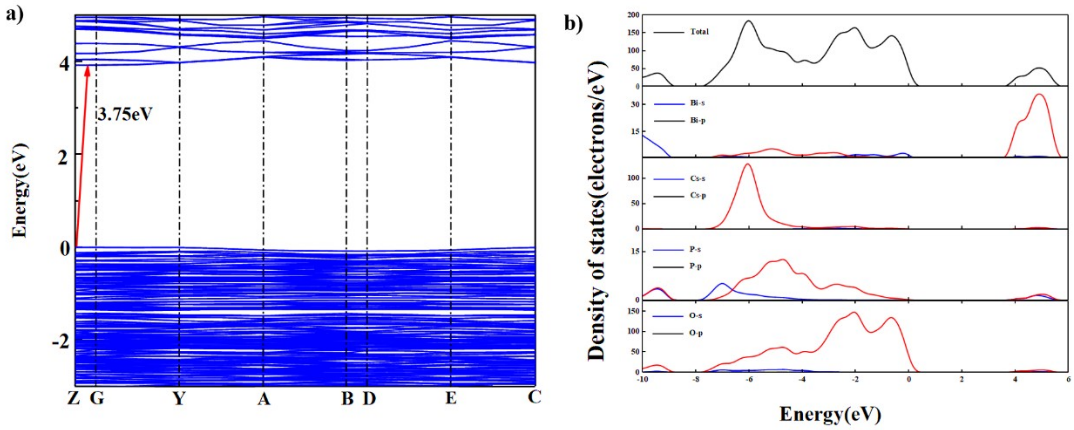

Figure S6. a) Band structure b) DOSs and total DOSs of $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$.

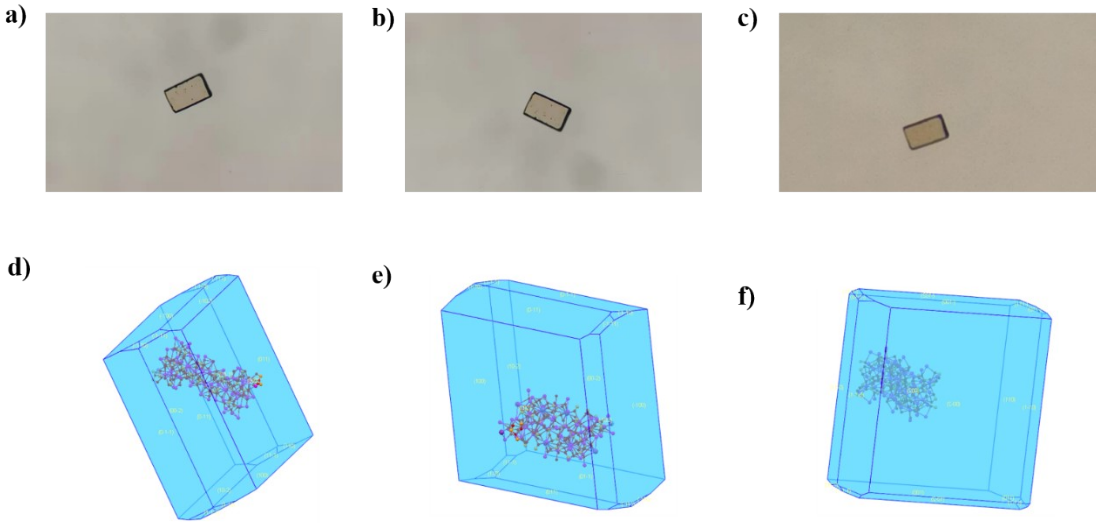

Figure S7. a-c) crystal photo and d-f) theoretical crystal morphology of $KCs_5Bi_4(PO_4)_2(P_2O_7)_3$, $RbCs_5Bi_4(PO_4)_2(P_2O_7)_3$ and $Cs_6Bi_4(PO_4)_2(P_2O_7)_3$, respectively.

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