Supporting Information

$Ba_2Bi_2[Zn(PO_4)_4]$: Ionic-Isolation-Activated First Barium Bismuth Zincophosphate with Unprecedented $_\infty[Zn(PO_4)_4]^{10-}$ Chains and Balanced Overall Performance

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters for BBZPO.

Atom	Wyck	Site	x/a	y/b	z/c	U [Å^2]
Bi1	8d	1	0.56166(3)	0.61306(2)	0.32924(2)	0.00777(11)
Ba1	8d	1	0.91275(5)	0.39142(3)	0.38812(4)	0.01142(13)
Zn1	4c	2	0.25455(14)	1/4	0.34571(12)	0.0138(3)
P3	4c	2	0.5928(3)	1/4	0.4322(2)	0.0066(5)
P2	4c	2	0.1337(3)	1/4	0.6015(2)	0.0094(6)
P1	8d	1	0.2677(2)	0.47664(12)	0.39393(17)	0.0079(4)
O7	4c	2	0.3044(9)	1/4	0.5917(8)	0.0222(19)
O1	8d	1	0.3990(6)	0.5100(4)	0.3126(5)	0.0192(13)
O6	4c	2	0.0743(8)	1/4	0.4579(7)	0.0133(16)
O10	4c	2	0.7418(8)	1/4	0.3546(6)	0.0098(15)
O9	8d	1	0.5921(6)	0.3317(3)	0.5166(5)	0.0176(13)
O2	8d	1	0.1310(6)	0.5330(3)	0.3740(5)	0.0144(12)
O8	4c	2	0.4706(9)	1/4	0.3299(7)	0.0179(18)
O3	8d	1	0.3031(6)	0.4791(3)	0.5404(4)	0.0162(12)
O4	8d	1	0.2345(6)	0.3880(3)	0.3418(5)	0.0143(12)
O5	8d	1	0.0820(8)	0.3304(5)	0.6671(6)	0.0400(19)

Table S2. Anisotropic displacement parameters, in $Å^2$, for atoms in BBZPO.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Bi1	0.00982(18)	0.00649(16)	0.00701(16)	0.00025(10)	-0.00027(10)	0.00029(10)
Ba1	0.0125(3)	0.0084(2)	0.0134(2)	0.00019(17)	-0.00197(16)	-0.00077(17)
Zn1	0.0108(7)	0.0161(7)	0.0146(6)	0.00000	0.0035(5)	0.00000
P3	0.0066(14)	0.0058(13)	0.0075(12)	0.00000	0.0013(9)	0.00000
P2	0.0116(16)	0.0091(13)	0.0075(12)	0.00000	0.0044(10)	0.00000
P1	0.0076(11)	0.0088(9)	0.0073(9)	0.0002(7)	-0.0004(7)	0.0005(7)
O7	0.008(5)	0.016(4)	0.043(5)	0.00000	-0.005(3)	0.00000
O1	0.018(3)	0.018(3)	0.021(3)	-0.006(2)	0.007(2)	0.000(2)
O6	0.017(5)	0.014(4)	0.008(3)	0.00000	-0.004(3)	0.00000
O10	0.004(4)	0.016(4)	0.009(3)	0.00000	-0.002(3)	0.00000
O9	0.021(3)	0.013(3)	0.018(3)	-0.003(2)	0.007(2)	-0.012(2)
O2	0.014(3)	0.015(3)	0.014(3)	0.006(2)	-0.002(2)	0.000(2)
O8	0.007(4)	0.031(5)	0.016(4)	0.00000	-0.003(3)	0.00000
O3	0.023(3)	0.022(3)	0.003(2)	0.007(2)	-0.001(2)	0.000(2)
O4	0.013(3)	0.010(3)	0.020(3)	-0.003(2)	0.005(2)	-0.002(2)
O5	0.059(5)	0.034(4)	0.027(4)	0.018(4)	0.008(3)	-0.016(3)

Table S3. Selected bond lengths for BBZPO.

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
Bi1—O7^{i}	2.5924(45)	Zn1—O8	1.9474(82)
Bi1—O1	2.1876(59)	Zn1—O4	2.1760(47)
Bi1—O9^{i}	2.2604(52)	P3—O10	1.5530(74)
Bi1—O3^{i}	2.3072(47)	P3—O9	1.5433(50)
Bi1—O5^{iii}	2.2722(68)	P3—O8	1.511(8)
Ba1—O6^{iv}	2.7467(42)	P2—O7	1.5366(85)
Ba1—O10	2.7223(42)	P2—O6	1.5521(74)
Ba1—O2^{iv}	2.9686(50)	P2—O5	1.5016(76)
Ba1—O2^{i}	2.7192(50)	P1—O1	1.5321(57)
Ba1—O3^{i}	2.9025(50)	P1—O2	1.5274(55)
Ba1—O4^{iv}	2.9287(54)	P1—O3	1.5208(45)
Zn1—O6	1.9795(73)	P1—O4	1.5194(51)

Table S4. Selected bond angles for BBZPO.

Atoms 1,2,3	Angle 1,2,3 [°]	Atoms 1,2,3	Angle 1,2,3 [°]
O1—Bi1—O7^{i}	161.480(155)	O8—Zn1—O4^{vi}	90.692(12)
O1—Bi1—O9^{i}	85.959(189)	O8—Zn1—O4	94.645(142)
O1—Bi1—O2^{ii}	118.954(142)	O7—P2—O6	106.396(427)
O1—Bi1—O3^{i}	86.067(192)	O5^{vi}—P2—O7	85.125(16)
O1—Bi1—O5^{iii}	81.612(233)	O5—P2—O7	109.715(274)
O9^{i}—Bi1—O7^{i}	75.561(123)	O5—P2—O6	108.063(237)
O9^{i}—Bi1—O2^{ii}	93.428(136)	O5^{vi}—P2—O6	104.167(14)
O9^{i}—Bi1—O3^{i}	99.540(173)	O5^{vi}—P2—O5	27.858(289)
O9^{i}—Bi1—O5^{iii}	90.241(212)	O2—P1—O1	110.439(307)
O2^{ii}—Bi1—O7^{i}	62.037(24)	O3—P1—O1	110.919(276)
O3^{i}—Bi1—O7^{i}	95.681(119)	O3—P1—O2	106.430(288)
O3^{i}—Bi1—O2^{ii}	33.813(118)	O4—P1—O1	106.085(318)
O5^{iii}—Bi1—O7^{i}	99.398(184)	O4—P1—O2	109.117(282)
O5^{iii}—Bi1—O2^{ii}	159.297(169)	O4—P1—O3	113.877(278)
O5^{iii}—Bi1—O3^{i}	163.694(205)	O10^{v}—Zn1—O4	94.207(138)
O6—Zn1—O10^{v}	102.416(213)	O10^{v}—Zn1—O4^{vi}	82.392(11)
O6—Zn1—O4^{vi}	83.835(12)	O8—Zn1—O6	149.609(320)
O6—Zn1—O4	86.720(139)	O8—Zn1—O10^{v}	47.193(237)

(i) 1-x, 1-y, 1-z; (ii) 1.5+x, y, 1.5-z; (iii) 0.5-x, 1-y, -0.5+z; (iv) 1+x, y, z;

(v) 0.5+x, y, 1.5-z; (vi) 0.5-x, 1.5+y, 0.5+z; (vii) -0.5-x, 1.5+y, 0.5+z; (viii) -1-x, 0.5+y, -z;

(ix) -1+x, y, z; (x) 1.5+x, -0.5-y, 1.5-z; (xi) 0.5-x, 1-y, 0.5+z.

Table S5. Calculated bond valence sum (BVS) for atoms in BBZPO.

Atom	BVS
Ba1	2.02
Bi1	3.19
Zn1	2.07
P1	5.46
P2	5.17
P3	4.97
O1	-2.31
O2	-2.08
O3	-2.05
O4	-1.98
O5	-1.98
O6	-2.24
O7	-1.87
O8	-2.03
O9	-1.86
O10	-2.21

Bond valence sums are calculated by using bond-valence theory ($S_i = \exp[(R_o - R_i)/B]$, where R_o is an empirical constant, R_i is the length of bond i (in angstroms), and B = 0.37).

Figure S1. IR Spectrum for BBZPO.