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Supporting Information

Synthesis, structure and magnetic property of a new organo-templated mixed-valent iron (II, III) borophosphate

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Table S1 Selected Bond Lengths [Å] and Angles [deg] for FeBPO-CJ28[a]

Fe(1)-O(24)	2.075(3)	O(22)-P(2)-O(18)	106.39(15)
Fe(1)-O(8)	2.117(3)	O(24)-P(3)-O(27)	115.07(16)
Fe(1)-O(6)	2.123(3)	O(24)-P(3)-O(29)	111.74(15)
Fe(1)-O(25)	2.124(3)	O(27)-P(3)-O(29)	106.98(15)
Fe(1)-O(26)	2.130(3)	O(24)-P(3)-O(12)	110.65(16)
Fe(1)-O(28	2.225(2)	O(27)-P(3)-O(12)	107.68(15)
Fe(2)-O(27)	1.958(3)	O(29)-P(3)-O(12)	104.05(15)
Fe(2)-O(17)	1.961(3)	O(26)-P(4)-O(17)#2	113.82(16)
Fe(2)-O(15)	1.985(3)	O(26)-P(4)-O(21)	111.57(16)
Fe(2)-O(20)	1.996(3)	O(17)#2-P(4)-O(21)	105.60(15)
Fe(2)-O(23)	2.017(3)	O(26)-P(4)-O(7)	110.13(17)
Fe(2)-O(19)	2.149(2)	O(17)#2-P(4)-O(7)	107.35(16)
P(1)-O(6)	1.491(3)	O(21)-P(4)-O(7)	108.09(17)
P(1)-O(30)	1.541(3)	O(8)#3-P(5)-O(15)	112.41(16)
P(1)-O(14)	1.549(3)	O(8)#3-P(5)-O(10)	108.69(16)
P(1)-O(11)	1.553(3)	O(15)-P(5)-O(10)	109.58(15)
P(2)-O(25)	1.506(3)	O(8)#3-P(5)-O(3)	109.95(16)
P(2)-O(20)#1	1.510(3)	O(15)-P(5)-O(3)	110.32(18)
P(2)-O(22)	1.563(3)	O(10)-P(5)-O(3)	105.66(18)
P(2)-O(18)	1.564(3)	O(4)-P(6)-O(5)	111.45(18)
P(3)-O(24)	1.497(3)	O(4)-P(6)-O(13)	112.81(17)
P(3)-O(27)	1.517(3)	O(5)-P(6)-O(13)	106.60(15)
P(3)-O(29)	1.563(3)	O(4)-P(6)-O(16)	113.13(17)
P(3)-O(12)	1.563(3)	O(5)-P(6)-O(16)	108.03(17)
P(4)-O(26)	1.497(3)	O(13)-P(6)-O(16)	104.34(14)
P(4)-O(17)#2	1.508(3)	O(2)-P(7)-O(23)	115.25(18)
P(4)-O(21)	1.558(3)	O(2)-P(7)-O(9)	110.99(18)
P(4)-O(7)	1.566(3)	O(23)-P(7)-O(9)	110.79(15)
P(5)-O(8)#3	1.499(3)	O(2)-P(7)-O(1)	109.9(2)
P(5)-O(15)	1.513(3)	O(23)-P(7)-O(1)	104.69(17)
P(5)-O(10)	1.562(3)	O(9)-P(7)-O(1)	104.44(17)
P(5)-O(3)	1.566(3)	O(28)-B(1)-O(16)	113.4(3)
P(6)-O(4)	1.493(3)	O(28)-B(1)-O(29)	112.8(3)
P(6)-O(5)	1.531(3)	O(16)-B(1)-O(29)	106.3(3)
P(6)-O(13)	1.558(3)	O(28)-B(1)-O(21)	109.8(3)
P(6)-O(16)	1.559(3)	O(16)-B(1)-O(21)	105.3(3)
P(7)-O(2)	1.493(3)	O(29)-B(1)-O(21)	108.9(3)
P(7)-O(23)	1.516(3)	O(28)-B(2)-O(22)	113.0(3)
P(7)-O(9)	1.560(3)	O(28)-B(2)-O(13)	112.9(3)
P(7)-O(1)	1.578(3)	O(22)-B(2)-O(13)	107.2(3)
B(1)-O(28)	1.449(5)	O(28)-B(2)-O(30)	111.9(3)

B(1)-O(16)	1.474(5)	O(22)-B(2)-O(30)	106.4(3)
B(1)-O(29)	1.476(5)	O(13)-B(2)-O(30)	105.0(3)
B(1)-O(21)	1.493(5)	O(19)-B(3)-O(12)	112.4(3)
B(2)-O(28)	1.430(5)	O(19)-B(3)-O(10)	110.4(3)
B(2)-O(22)	1.472(5)	O(12)-B(3)-O(10)	110.3(3)
B(2)-O(13)	1.478(5)	O(19)-B(3)-O(14)#4	113.2(3)
B(2)-O(30)	1.505(5)	O(12)-B(3)-O(14)#4	102.4(3)
B(3)-O(19)	1.461(4)	O(10)-B(3)-O(14)#4	107.7(3)
B(3)-O(12)	1.468(5)	O(19)-B(4)-O(9)	110.4(3)
B(3)-O(10)	1.471(5)	O(19)-B(4)-O(11)#4	113.8(3)
B(3)-O(14)#4	1.481(5)	O(9)-B(4)-O(11)#4	107.6(3)
B(4)-O(19)	1.461(4)	O(19)-B(4)-O(18)#5	112.3(3)
B(4)-O(9)	1.472(5)	O(9)-B(4)-O(18)#5	110.9(3)
B(4)-O(11)#4	1.475(4)	O(11)#4-B(4)-O(18)#5	101.5(3)
B(4)-O(18)#5	1.480(5)	P(7)-O(1)-H(1)	109.5
O(1)-H(1)	0.82	P(5)-O(3)-H(3)	109.5
O(3)-H(3)	0.82	P(6)-O(5)-H(5)	109.5
O(5)-H(5)	0.82	P(1)-O(6)-Fe(1)	127.63(16)
O(7)-H(7)	0.82	P(4)-O(7)-H(7)	109.5
O(8)-P(5)#3	1.499(3)	P(5)#3-O(8)-Fe(1)	136.89(17)
O(11)-B(4)#6	1.475(4)	B(4)-O(9)-P(7)	128.5(2)
O(14)-B(3)#6	1.481(5)	B(3)-O(10)-P(5)	127.3(2)
O(17)-P(4)#7	1.508(3)	B(4)#6-O(11)-P(1)	128.7(2)
O(18)-B(4)#1	1.480(5)	B(3)-O(12)-P(3)	132.1(2)
O(20)-P(2)#5	1.510(3)	B(2)-O(13)-P(6)	122.6(2)
C(1)-C(2)	1.463(7)	B(3)#6-O(14)-P(1)	126.7(2)
C(1)-N(1)	1.472(8)	P(5)-O(15)-Fe(2)	135.44(17)
C(1)-H(1A)	0.97	B(1)-O(16)-P(6)	121.4(2)
C(1)-H(1B)	0.97	P(4)#7-O(17)-Fe(2)	154.44(19)
C(2)-N(2)	1.522(6)	B(4)#1-O(18)-P(2)	131.7(2)
C(2)-H(2A)	0.97	B(3)-O(19)-B(4)	125.4(3)
C(2)-H(2B)	0.97	B(3)-O(19)-Fe(2)	117.3(2)
C(3)-N(2)	1.469(6)	B(4)-O(19)-Fe(2)	117.3(2)
C(3)-C(4)	1.501(6)	P(2)#5-O(20)-Fe(2)	132.28(16)
C(3)-H(3A)	0.97	B(1)-O(21)-P(4)	128.5(2)
C(3)-H(3B)	0.97	B(2)-O(22)-P(2)	131.5(2)
C(4)-N(3)	1.487(6)	P(7)-O(23)-Fe(2)	131.44(17)
C(4)-H(4A)	0.97	P(3)-O(24)-Fe(1)	129.53(16)
C(4)-H(4B)	0.97	P(2)-O(25)-Fe(1)	128.88(15)
C(5)-C(6)	1.508(14)	P(4)-O(26)-Fe(1)	124.79(16)
C(5)-N(4)	1.499(12)	P(3)-O(27)-Fe(2)	131.77(16)
C(5')-C(6')	1.548(17)	B(2)-O(28)-B(1)	125.2(3)

C(5')-N(4)#8	1.481(13)	B(2)-O(28)-Fe(1)	115.7(2)
C(6)-N(5)	1.496(13)	B(1)-O(28)-Fe(1)	113.7(2)
C(6')-N(5')	1.387(17)	B(1)-O(29)-P(3)	129.1(2)
N(1)-H(1C)	0.89	B(2)-O(30)-P(1)	127.8(2)
N(1)-H(1D)	0.89	C(2)-C(1)-N(1)	115.0(5)
N(1)-H(1E)	0.89	C(2)-C(1)-H(1A)	108.5
N(2)-H(2C)	0.9	N(1)-C(1)-H(1A)	108.5
N(2)-H(2D)	0.9	C(2)-C(1)-H(1B)	108.5
N(3)-H(3C)	0.89	N(1)-C(1)-H(1B)	108.5
N(3)-H(3D)	0.89	H(1A)-C(1)-H(1B)	107.5
N(3)-H(3E)	0.89	C(1)-C(2)-N(2)	114.5(4)
O(24)-Fe(1)-O(8)	91.38(10)	C(1)-C(2)-H(2A)	108.6
O(24)-Fe(1)-O(6)	90.08(11)	N(2)-C(2)-H(2A)	108.6
O(8)-Fe(1)-O(6)	93.96(11)	C(1)-C(2)-H(2B)	108.6
O(24)-Fe(1)-O(25)	178.00(11)	N(2)-C(2)-H(2B)	108.6
O(8)-Fe(1)-O(25)	89.67(10)	H(2A)-C(2)-H(2B)	107.6
O(6)-Fe(1)-O(25)	91.52(11)	N(2)-C(3)-C(4)	113.5(4)
O(24)-Fe(1)-O(26)	88.85(11)	N(2)-C(3)-H(3A)	108.9
O(8)-Fe(1)-O(26)	90.72(11)	C(4)-C(3)-H(3A)	108.9
O(6)-Fe(1)-O(26)	175.23(10)	N(2)-C(3)-H(3B)	108.9
O(25)-Fe(1)-O(26)	89.45(11)	C(4)-C(3)-H(3B)	108.9
O(24)-Fe(1)-O(28)	93.49(10)	H(3A)-C(3)-H(3B)	107.7
O(8)-Fe(1)-O(28)	173.15(10)	N(3)-C(4)-C(3)	110.4(4)
O(6)-Fe(1)-O(28)	90.84(10)	N(3)-C(4)-H(4A)	109.6
O(25)-Fe(1)-O(28)	85.32(9)	C(3)-C(4)-H(4A)	109.6
O(26)-Fe(1)-O(28)	84.58(10)	N(3)-C(4)-H(4B)	109.6
O(27)-Fe(2)-O(17)	92.60(11)	C(3)-C(4)-H(4B)	109.6
O(27)-Fe(2)-O(15)	92.10(12)	H(4A)-C(4)-H(4B)	108.1
O(17)-Fe(2)-O(15)	91.92(11)	N(4)-C(5)-C(6)	110.8(8)
O(27)-Fe(2)-O(20)	177.65(11)	C(6')-C(5')-N(4)#8	105.4(9)
O(17)-Fe(2)-O(20)	86.86(11)	N(5)-C(6)-C(5)	113.5(8)
O(15)-Fe(2)-O(20)	90.20(11)	C(5')-C(6)-N(5')	118.1(11)
O(27)-Fe(2)-O(23)	90.30(11)	C(1)-N(1)-H(1C)	109.5
O(17)-Fe(2)-O(23)	98.47(11)	C(1)-N(1)-H(1D)	109.5
O(15)-Fe(2)-O(23)	169.21(11)	H(1C)-N(1)-H(1D)	109.5
O(20)-Fe(2)-O(23)	87.52(11)	C(1)-N(1)-H(1E)	109.5
O(27)-Fe(2)-O(19)	90.30(10)	H(1C)-N(1)-H(1E)	109.5
O(17)-Fe(2)-O(19)	174.57(11)	H(1D)-N(1)-H(1E)	109.5
O(15)-Fe(2)-O(19)	83.37(10)	C(3)-N(2)-C(2)	109.9(4)
O(20)-Fe(2)-O(19)	90.43(10)	C(3)-N(2)-H(2C)	109.7
O(23)-Fe(2)-O(19)	86.11(10)	C(2)-N(2)-H(2C)	109.7
O(6)-P(1)-O(30)	112.61(15)	C(3)-N(2)-H(2D)	109.7

O(6)-P(1)-O(14)	113.50(16)	C(2)-N(2)-H(2D)	109.7
O(30)-P(1)-O(14)	107.93(15)	H(2C)-N(2)-H(2D)	108.2
O(6)-P(1)-O(11)	113.21(15)	C(4)-N(3)-H(3C)	109.5
O(30)-P(1)-O(11)	103.55(14)	C(4)-N(3)-H(3D)	109.5
O(14)-P(1)-O(11)	105.28(14)	H(3C)-N(3)-H(3D)	109.5
O(25)-P(2)-O(20)#1	114.06(15)	C(4)-N(3)-H(3E)	109.5
O(25)-P(2)-O(22)	110.41(15)	H(3C)-N(3)-H(3E)	109.5
O(20)#1-P(2)-O(22)	107.63(15)	H(3D)-N(3)-H(3E)	109.5
O(25)-P(2)-O(18)	108.51(15)	C(5)-N(4)-C(5)#8	141.7(8)
O(20)#1-P(2)-O(18)	109.57(14)	C(5')#8-N(4)-C(5)	115.9(6)

[a]Symmetry transformations used to generate equivalent atoms: #1 x-1,y-1,z; #2 x-1,y,z; #3 -x+2,-y+2,-z+1; #4 x,y+1,z; #5 x+1,y+1,z; #6 x,y-1,z; #7 x+1,y,z; #8 -x+1,-y+2,-z+1

Table S2 Hydrogen bonds for FeBPO-CJ28[a]

D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (^{o})
O(1)-H(1)...O(5)#9	0.82	2.03	2.804(4)	156.1
O(5)-H(5)...O(1)#9	0.82	2.07	2.804(4)	149.1
O(7)-H(7)...O(18)	0.82	2.06	2.729(4)	138.9
N(1)-H(1C)...O(11)#10	0.89	2.08	2.929(5)	159.5
N(1)-H(1D)...O(4)#10	0.89	1.91	2.779(6)	165.6
N(1)-H(1E)...O(5)	0.89	2.26	3.127(6)	163.9
N(2)-H(2C)...O(2)#10	0.9	1.79	2.667(5)	163.6
N(2)-H(2D)...O(4)#10	0.9	1.9	2.790(5)	168.9
N(3)-H(3C)...O(21)#6	0.89	2.08	2.809(4)	138.3
N(3)-H(3D)...O(22)	0.89	2.08	2.931(4)	158.9
N(3)-H(3E)...O(12)#6	0.89	2.1	2.940(4)	156.3
N(3)-H(3E)...O(14)	0.89	2.32	3.041(4)	137.8

[a]Symmetry transformations used to generate equivalent atoms:

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

#4 x,y+1,z #5 x+1,y+1,z #6 x,y-1,z #7 x+1,y,z

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

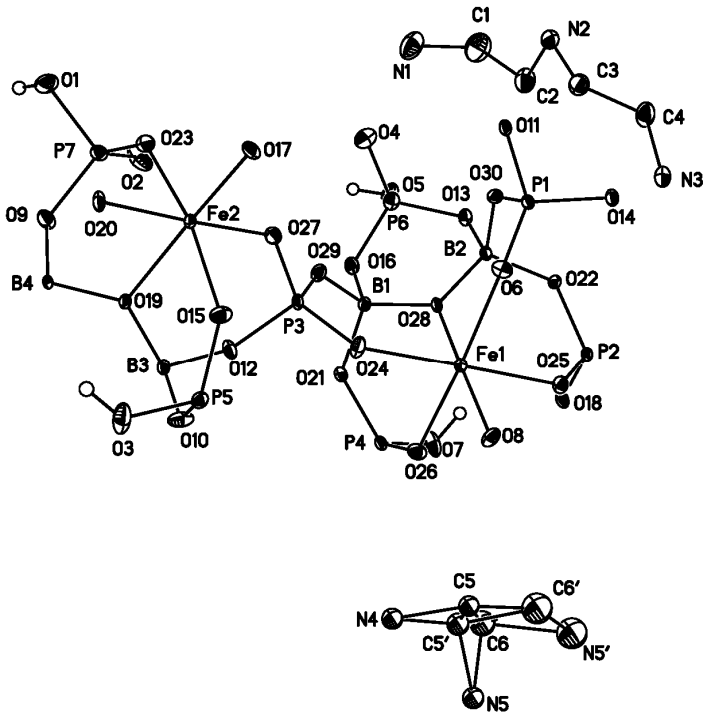

Figure S1 Thermal ellipsoid plots (30% probability) and atomic labeling schemes of the framework in FeBPO-CJ28.

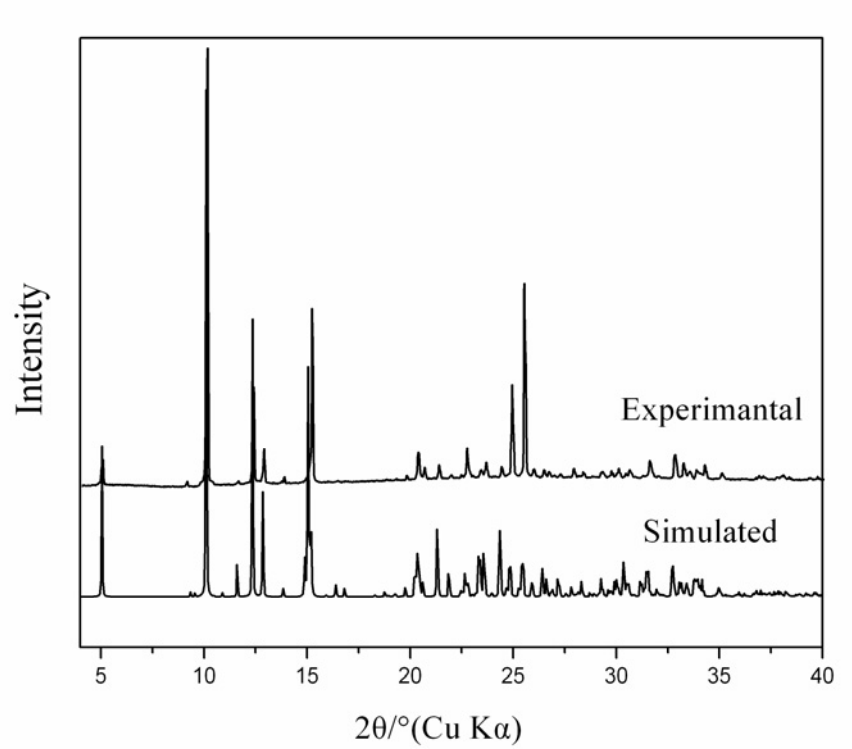

Figure S2 Simulated and experimental powder X-ray diffraction patterns of FeBPO-CJ28.

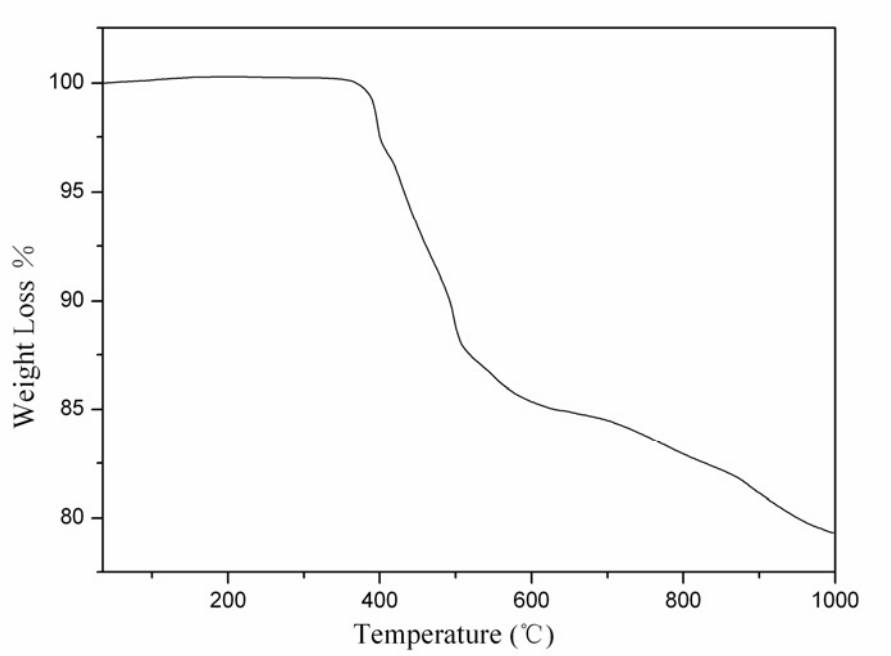

Figure S3 TG curve of FeBPO-CJ28. Restrained to the experimental condition, the temperature can only come to 1000 ^{o}C, and the total loss weight about 20.7% is a little smaller than the calculated value (22.2%).