Electronic Supplementary Information for Dalton Transactions

Supporting Information

$(NH_4)_6[Mn_3B_6P_9O_{36}(OH)_3]\cdot 4H_2O$: A New Open-Framework Manganese Borophosphate Synthesized by Using Boric Acid Flux Method

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Table S1 Selected Bond Lengths [Å] and Angles [deg] for MnBPO-CJ31[a].

Mn(1)-O(8)	2.104(4)	O(18)-Mn(3)-O(27)	99.05(19)
Mn(1)-O(6)	2.117(4)	O(18)-Mn(3)-O(19)	90.42(18)
Mn(1)-O(5)	2.137(4)	O(27)-Mn(3)-O(19)	88.84(17)
Mn(1)-O(3)	2.151(4)	O(18)-Mn(3)-O(21)	89.82(18)
Mn(1)-O(12)	2.213(4)	O(27)-Mn(3)-O(21)	93.12(19)
Mn(1)-O(13)	2.417(4)	O(19)-Mn(3)-O(21)	177.96(19)
Mn(2)-O(38)	2.142(4)	O(18)-Mn(3)-O(16)	97.35(19)
Mn(2)-O(34)	2.146(4)	O(27)-Mn(3)-O(16)	163.56(16)
Mn(2)-O(23)	2.165(4)	O(19)-Mn(3)-O(16)	92.10(16)
Mn(2)-O(37)	2.202(4)	O(21)-Mn(3)-O(16)	85.86(18)
Mn(2)-O(31)	2.231(4)	O(18)-Mn(3)-O(20)	177.89(18)
Mn(2)-O(39)	2.297(4)	O(27)-Mn(3)-O(20)	81.48(15)
Mn(3)-O(18)	2.079(5)	O(19)-Mn(3)-O(20)	91.63(15)
Mn(3)-O(27)	2.147(4)	O(21)-Mn(3)-O(20)	88.11(15)
Mn(3)-O(19)	2.151(4)	O(16)-Mn(3)-O(20)	82.09(14)
Mn(3)-O(21)	2.174(5)	O(8)#1-P(1)-O(8)	113.9(3)
Mn(3)-O(16)	2.182(4)	O(8)#1-P(1)-O(9)	106.1(2)
Mn(3)-O(20)	2.290(4)	O(8)-P(1)-O(9)	112.3(2)
P(1)-O(8)#1	1.517(4)	O(8)#1-P(1)-O(9)#1	112.3(2)
P(1)-O(8)	1.517(4)	O(8)-P(1)-O(9)#1	106.1(2)
P(1)-O(9)	1.564(4)	O(9)-P(1)-O(9)#1	106.0(3)
P(1)-O(9)#1	1.564(4)	O(38)-P(2)-O(12)	115.0(2)
P(2)-O(38)	1.512(4)	O(38)-P(2)-O(11)	109.9(2)
P(2)-O(12)	1.516(4)	O(12)-P(2)-O(11)	110.7(2)
P(2)-O(11)	1.570(4)	O(38)-P(2)-O(10)	107.1(2)
P(2)-O(10)	1.591(4)	O(12)-P(2)-O(10)	109.7(2)
P(3)-O(6)	1.513(4)	O(11)-P(2)-O(10)	103.8(2)
P(3)-O(6)#2	1.513(4)	O(6)-P(3)-O(6)#2	113.0(4)
P(3)-O(7)#2	1.568(4)	O(6)-P(3)-O(7)#2	110.8(2)
P(3)-O(7)	1.568(4)	O(6)#2-P(3)-O(7)#2	106.9(2)
P(4)-O(16)	1.501(4)	O(6)-P(3)-O(7)	106.9(2)
P(4)-O(15)	1.552(4)	O(6)#2-P(3)-O(7)	110.8(2)
P(4)-O(14)	1.563(4)	O(7)#2-P(3)-O(7)	108.3(3)
P(4)-O(17)	1.572(4)	O(16)-P(4)-O(15)	110.8(2)
P(5)-O(31)	1.490(4)	O(16)-P(4)-O(14)	110.8(2)
P(5)-O(26)	1.547(4)	O(15)-P(4)-O(14)	105.7(2)
P(5)-O(30)	1.555(4)	O(16)-P(4)-O(17)	114.0(2)
P(5)-O(25)	1.562(4)	O(15)-P(4)-O(17)	107.5(2)
P(6)-O(21)	1.494(4)	O(14)-P(4)-O(17)	107.6(2)
P(6)-O(23)	1.510(4)	O(31)-P(5)-O(26)	110.8(2)

P(6)-O(24)	1.568(5)	O(31)-P(5)-O(30)	113.0(2)
P(6)-O(22)	1.568(4)	O(26)-P(5)-O(30)	106.3(2)
P(7)-O(19)#3	1.514(4)	O(31)-P(5)-O(25)	112.2(2)
P(7)-O(34)	1.519(4)	O(26)-P(5)-O(25)	105.9(2)
P(7)-O(33)	1.558(4)	O(30)-P(5)-O(25)	108.3(2)
P(7)-O(32)	1.581(4)	O(21)-P(6)-O(23)	113.9(3)
P(8)-O(3)	1.492(4)	O(21)-P(6)-O(24)	110.1(4)
P(8)-O(1)	1.546(4)	O(23)-P(6)-O(24)	110.7(2)
P(8)-O(2)	1.556(4)	O(21)-P(6)-O(22)	109.7(2)
P(8)-O(4)	1.567(4)	O(23)-P(6)-O(22)	107.2(2)
P(9)-O(5)#4	1.506(5)	O(24)-P(6)-O(22)	104.9(3)
P(9)-O(27)	1.506(4)	O(19)#3-P(7)-O(34)	114.6(2)
P(9)-O(29)	1.582(4)	O(19)#3-P(7)-O(33)	110.8(2)
P(9)-O(28)	1.602(5)	O(34)-P(7)-O(33)	108.9(2)
P(10)-O(18)#5	1.488(5)	O(19)#3-P(7)-O(32)	109.9(2)
P(10)-O(37)	1.498(5)	O(34)-P(7)-O(32)	109.4(2)
P(10)-O(36)	1.549(5)	O(33)-P(7)-O(32)	102.6(2)
P(10)-O(35)	1.596(6)	O(3)-P(8)-O(1)	110.2(2)
B(1)-O(13)	1.452(7)	O(3)-P(8)-O(2)	112.0(3)
B(1)-O(9)	1.459(7)	O(1)-P(8)-O(2)	108.3(2)
B(1)-O(10)	1.487(7)	O(3)-P(8)-O(4)	113.7(3)
B(1)-O(14)#1	1.518(7)	O(1)-P(8)-O(4)	105.2(2)
B(2)-O(7)#2	1.448(7)	O(2)-P(8)-O(4)	107.0(2)
B(2)-O(13)	1.460(6)	O(5)#4-P(9)-O(27)	116.6(3)
B(2)-O(15)#1	1.501(7)	O(5)#4-P(9)-O(29)	106.5(2)
B(2)-O(11)	1.511(7)	O(27)-P(9)-O(29)	111.6(2)
B(3)-O(20)#3	1.451(7)	O(5)#4-P(9)-O(28)	107.0(3)
B(3)-O(29)#3	1.476(7)	O(27)-P(9)-O(28)	108.3(3)
B(3)-O(33)	1.494(7)	O(29)-P(9)-O(28)	106.3(2)
B(3)-O(26)#6	1.496(6)	O(18)#5-P(10)-O(37)	117.3(3)
B(4)-O(39)	1.450(7)	O(18)#5-P(10)-O(36)	105.2(3)
B(4)-O(32)	1.479(7)	O(37)-P(10)-O(36)	111.8(3)
B(4)-O(2)#7	1.492(7)	O(18)#5-P(10)-O(35)	106.7(3)
B(4)-O(30)	1.496(7)	O(37)-P(10)-O(35)	108.7(3)
B(5)-O(36)	1.439(8)	O(36)-P(10)-O(35)	106.6(4)
B(5)-O(39)	1.441(7)	O(13)-B(1)-O(9)	112.3(4)
B(5)-O(1)#7	1.467(7)	O(13)-B(1)-O(10)	111.0(4)
B(5)-O(24)	1.469(8)	O(9)-B(1)-O(10)	110.6(4)
B(6)-O(20)	1.429(7)	O(13)-B(1)-O(14)#1	110.3(4)
B(6)-O(22)	1.467(7)	O(9)-B(1)-O(14)#1	105.4(4)
B(6)-O(25)#5	1.480(7)	O(10)-B(1)-O(14)#1	106.9(4)
B(6)-O(17)	1.496(7)	O(7)#2-B(2)-O(13)	111.0(4)

O(8)-Mn(1)-O(6)	176.13(18)	O(7)#2-B(2)-O(15)#1	104.9(4)
O(8)-Mn(1)-O(5)	91.11(17)	O(13)-B(2)-O(15)#1	110.3(4)
O(6)-Mn(1)-O(5)	88.29(17)	O(7)#2-B(2)-O(11)	113.8(4)
O(8)-Mn(1)-O(3)	91.07(17)	O(13)-B(2)-O(11)	108.4(4)
O(6)-Mn(1)-O(3)	92.70(18)	O(15)#1-B(2)-O(11)	108.4(4)
O(5)-Mn(1)-O(3)	85.47(17)	O(20)#3-B(3)-O(29)#3	109.8(4)
O(8)-Mn(1)-O(12)	88.73(16)	O(20)#3-B(3)-O(33)	113.1(4)
O(6)-Mn(1)-O(12)	88.01(17)	O(29)#3-B(3)-O(33)	109.6(4)
O(5)-Mn(1)-O(12)	113.57(16)	O(20)#3-B(3)-O(26)#6	113.0(4)
O(3)-Mn(1)-O(12)	160.96(16)	O(29)#3-B(3)-O(26)#6	108.0(4)
O(8)-Mn(1)-O(13)	86.54(14)	O(33)-B(3)-O(26)#6	103.0(4)
O(6)-Mn(1)-O(13)	94.85(15)	O(39)-B(4)-O(32)	114.0(4)
O(5)-Mn(1)-O(13)	167.59(15)	O(39)-B(4)-O(2)#7	112.6(4)
O(3)-Mn(1)-O(13)	82.40(15)	O(32)-B(4)-O(2)#7	102.6(4)
O(12)-Mn(1)-O(13)	78.59(14)	O(39)-B(4)-O(30)	110.9(4)
O(38)-Mn(2)-O(34)	88.16(16)	O(32)-B(4)-O(30)	106.9(4)
O(38)-Mn(2)-O(23)	94.93(16)	O(2)#7-B(4)-O(30)	109.4(4)
O(34)-Mn(2)-O(23)	175.95(16)	O(36)-B(5)-O(39)	112.1(5)
O(38)-Mn(2)-O(37)	101.75(16)	O(36)-B(5)-O(1)#7	106.2(5)
O(34)-Mn(2)-O(37)	88.86(17)	O(39)-B(5)-O(1)#7	113.1(4)
O(23)-Mn(2)-O(37)	87.96(17)	O(36)-B(5)-O(24)	109.5(6)
O(38)-Mn(2)-O(31)	97.00(16)	O(39)-B(5)-O(24)	112.6(5)
O(34)-Mn(2)-O(31)	94.20(16)	O(1)#7-B(5)-O(24)	102.8(5)
O(23)-Mn(2)-O(31)	88.03(16)	O(20)-B(6)-O(22)	114.4(4)
O(37)-Mn(2)-O(31)	161.10(16)	O(20)-B(6)-O(25)#5	112.2(4)
O(38)-Mn(2)-O(39)	174.72(15)	O(22)-B(6)-O(25)#5	103.6(4)
O(34)-Mn(2)-O(39)	90.92(14)	O(20)-B(6)-O(17)	110.0(4)
O(23)-Mn(2)-O(39)	86.24(14)	O(22)-B(6)-O(17)	108.8(4)
O(37)-Mn(2)-O(39)	83.43(15)	O(25)#5-B(6)-O(17)	107.6(4)
O(31)-Mn(2)-O(39)	77.88(15)		

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

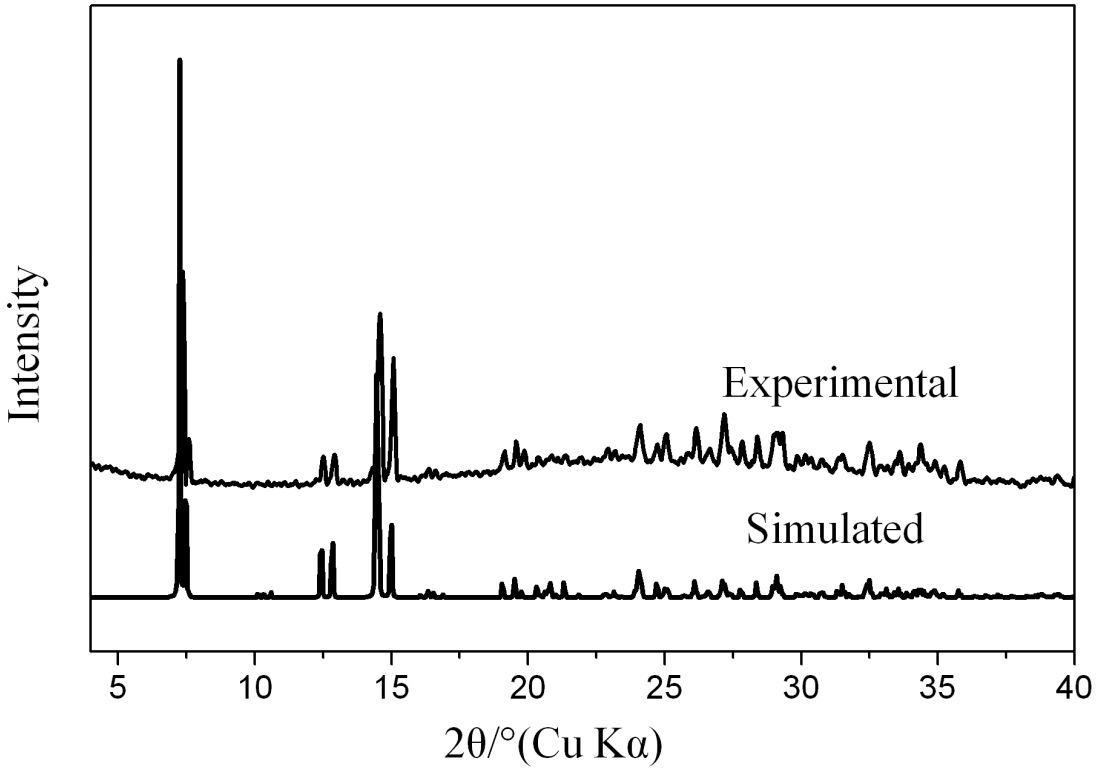

Figure S1 Simulated and experimental powder X-ray diffraction patterns of MnBPO-CJ31.

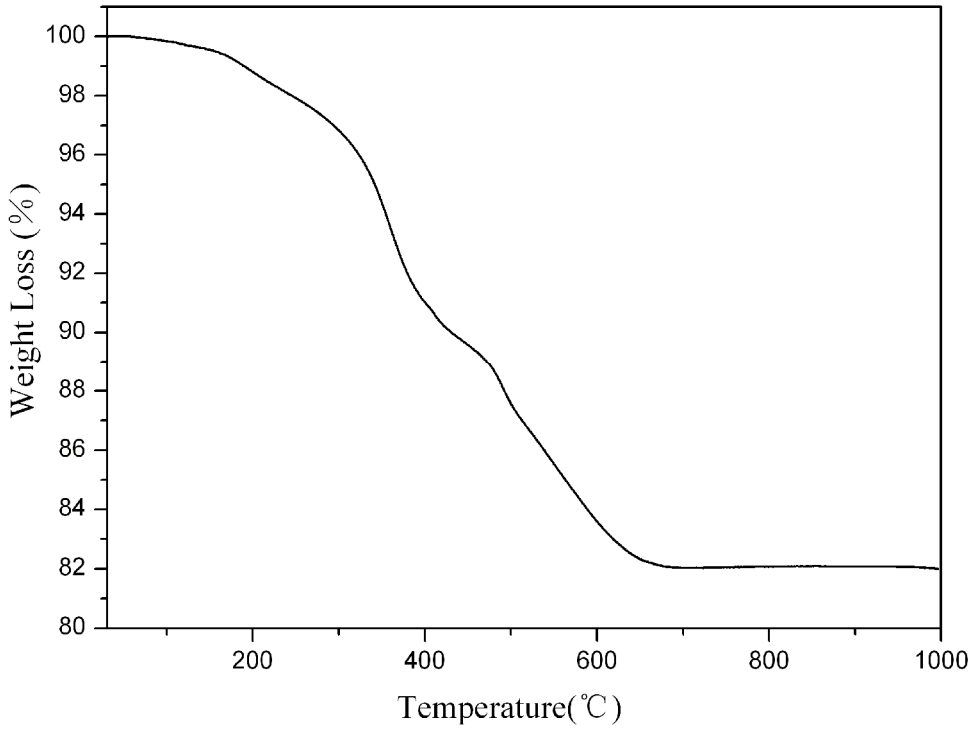

Figure S2 TG curve of MnBPO-CJ31.

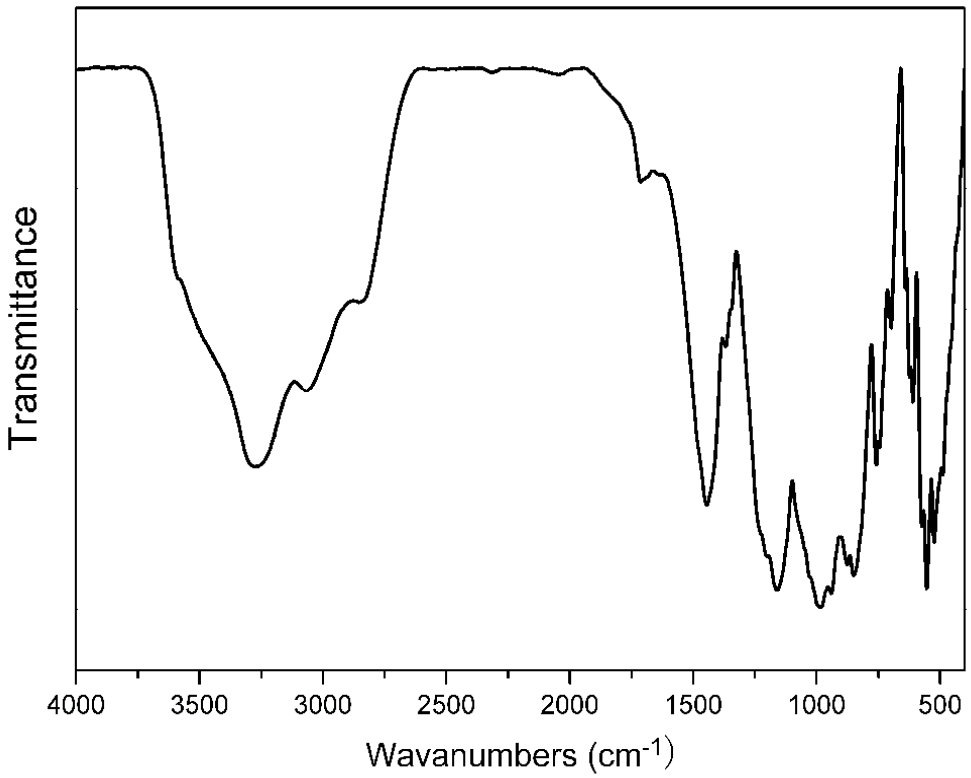

Figure S3 Infrared Spectrum of MnBPO-CJ31.

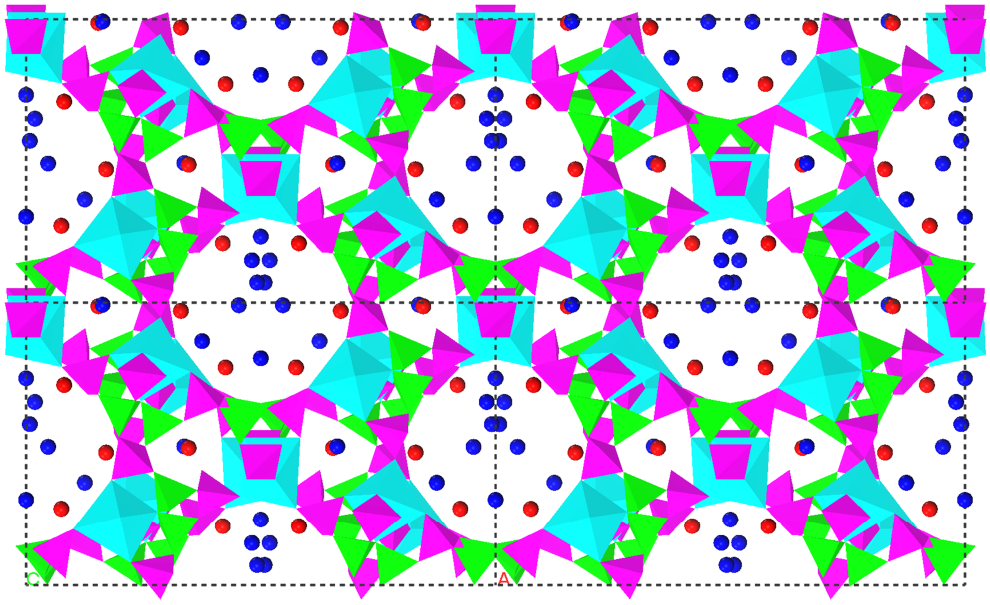

Fig. S4 The location of N (NH_4^+) and Ow (H_2O) in the framework of MnBPO-CJ31 along the [001] direction. Color code: Mn, bright blue; P, purple; B, green; N, blue sphere; Ow, red sphere.