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SUPPLEMENTARY MATERIAL

Table VII. Bond Distances (Å) and Angles (deg) for $[\text{Fe}_2^{\text{III}}(\text{BBPMP})$
 $(\mu\text{-OAc})_2]\text{ClO}_4 \cdot \text{H}_2\text{O}$.

Fe(1) - O(1)	2.054(8)
Fe(1) - O(2)	1.851(9)
Fe(1) - O(4)	1.965(8)
Fe(1) - O(6)	1.980(9)
Fe(1) - N(1)	2.18(1)
Fe(1) - N(2)	2.13(1)
Fe(2) - O(1)	2.055(7)
Fe(2) - O(3)	1.861(8)
Fe(2) - O(5)	1.993(9)
Fe(2) - O(7)	1.956(9)
Fe(2) - N(3)	2.17(1)
Fe(2) - N(4)	2.13(1)
Fe(1)...Fe(2)	3.528(8)
O(1) - C(1)	1.34(1)
O(2) - C(21)	1.33(2)
O(3) - C(35)	1.30(2)
O(4) - C(36)	1.24(1)
O(5) - C(36)	1.25(1)

O(6)	-	C(38)	1.24(2)
O(7)	-	C(38)	1.22(2)
N(1)	-	C(8)	1.46(2)
N(1)	-	C(9)	1.53(2)
N(1)	-	C(15)	1.51(2)
N(2)	-	C(10)	1.28(2)
N(2)	-	C(14)	1.36(2)
N(3)	-	C(22)	1.48(2)
N(3)	-	C(23)	1.49(2)
N(3)	-	C(29)	1.51(2)
N(4)	-	C(24)	1.33(2)
N(4)	-	C(28)	1.37(2)
C(1)	-	C(2)	1.34(2)
C(1)	-	C(6)	1.37(2)
C(2)	-	C(3)	1.43(2)
C(2)	-	C(8)	1.47(2)
C(3)	-	C(4)	1.35(2)
C(4)	-	C(5)	1.36(2)
C(4)	-	C(7)	1.48(2)
C(5)	-	C(6)	1.42(2)
C(6)	-	C(22)	1.47(2)
C(9)	-	C(10)	1.45(2)
C(10)	-	C(11)	1.41(2)
C(11)	-	C(12)	1.36(2)

C(12)	-	C(13)	1.37(2)
C(13)	-	C(14)	1.38(2)
C(15)	-	C(16)	1.50(2)
C(16)	-	C(17)	1.39(2)
C(16)	-	C(21)	1.35(2)
C(17)	-	C(18)	1.37(2)
C(18)	-	C(19)	1.34(2)
C(19)	-	C(20)	1.36(2)
C(20)	-	C(21)	1.41(2)
C(23)	-	C(24)	1.48(2)
C(24)	-	C(25)	1.35(2)
C(25)	-	C(26)	1.40(2)
C(26)	-	C(27)	1.35(2)
C(27)	-	C(28)	1.37(2)
C(29)	-	C(30)	1.47(2)
C(30)	-	C(31)	1.38(2)
C(30)	-	C(35)	1.37(2)
C(31)	-	C(32)	1.37(2)
C(32)	-	C(33)	1.39(2)
C(33)	-	C(34)	1.35(2)
C(34)	-	C(35)	1.43(2)
C(36)	-	C(37)	1.44(2)
C(38)	-	C(39)	1.48(2)

Cl	-	O(8)	1.40(2)
Cl	-	O(9)	1.30(2)
Cl	-	O(10)	1.31(2)
Cl	-	O(11)	1.42(2)
Cl	-	O(8)'	1.64(3)
Cl	-	O(9)'	1.49(3)
Cl	-	O(10)'	1.50(3)
Cl	-	O(11)'	1.44(4)

O(1)	-	Fe(1)	-	O(2)	176.3(3)
O(1)	-	Fe(1)	-	O(4)	91.0(3)
O(1)	-	Fe(1)	-	O(6)	88.8(3)
O(1)	-	Fe(1)	-	N(1)	87.7(3)
O(1)	-	Fe(1)	-	N(2)	85.6(3)
O(2)	-	Fe(1)	-	O(4)	92.6(4)
O(2)	-	Fe(1)	-	O(6)	91.7(4)
O(2)	-	Fe(1)	-	N(1)	88.6(4)
O(2)	-	Fe(1)	-	N(2)	93.5(4)
O(4)	-	Fe(1)	-	O(6)	97.6(4)
O(4)	-	Fe(1)	-	N(1)	169.3(4)
O(4)	-	Fe(1)	-	N(2)	90.5(4)
O(6)	-	Fe(1)	-	N(1)	92.9(4)
O(6)	-	Fe(1)	-	N(2)	170.2(4)
N(1)	-	Fe(1)	-	N(2)	78.9(4)

O(1)	-	Fe(2)	-	O(3)	175.3(3)
O(1)	-	Fe(2)	-	O(5)	86.5(3)
O(1)	-	Fe(2)	-	O(7)	91.7(3)
O(1)	-	Fe(2)	-	N(3)	87.0(3)
O(1)	-	Fe(2)	-	N(4)	85.2(3)
O(3)	-	Fe(2)	-	O(5)	93.3(4)
O(3)	-	Fe(2)	-	O(7)	93.0(4)
O(3)	-	Fe(2)	-	N(3)	88.3(4)
O(3)	-	Fe(2)	-	N(4)	93.9(4)
O(5)	-	Fe(2)	-	O(7)	97.9(3)
O(5)	-	Fe(2)	-	N(3)	89.8(4)
O(5)	-	Fe(2)	-	N(4)	165.5(4)
O(7)	-	Fe(2)	-	N(3)	172.1(4)
O(7)	-	Fe(2)	-	N(4)	94.2(4)
N(3)	-	Fe(2)	-	N(4)	77.8(4)
Fe(1)	-	O(1)	-	Fe(2)	118.3(4)
Fe(1)	-	O(4)	-	O(5)	107.5(4)
Fe(2)	-	O(5)	-	O(4)	111.9(4)
Fe(1)	-	O(6)	-	O(7)	111.8(5)
Fe(2)	-	O(7)	-	O(6)	109.0(4)
C(8)	-	N(1)	-	C(9)	109.3(9)
C(8)	-	N(1)	-	C(15)	107.4(9)

C(9)	-	N(1)	-	C(15)	111.7(9)
C(10)	-	N(2)	-	C(14)	119.(1)
C(22)	-	N(3)	-	C(23)	111.3(9)
C(22)	-	N(3)	-	C(29)	107.1(9)
C(23)	-	N(3)	-	C(29)	109.7(9)
C(24)	-	N(4)	-	C(28)	115.(1)
O(1)	-	C(1)	-	C(2)	120.(1)
O(1)	-	C(1)	-	C(6)	117.(1)
C(2)	-	C(1)	-	C(6)	123.(1)
C(1)	-	C(2)	-	C(3)	118.(1)
C(1)	-	C(2)	-	C(8)	123.(1)
C(3)	-	C(2)	-	C(8)	119.(1)
C(2)	-	C(3)	-	C(4)	120.(1)
C(3)	-	C(4)	-	C(5)	121.(1)
C(3)	-	C(4)	-	C(7)	119.(1)
C(5)	-	C(4)	-	C(7)	119.(1)
C(4)	-	C(5)	-	C(6)	119.(1)
C(1)	-	C(6)	-	C(5)	119.(1)
C(1)	-	C(6)	-	C(22)	122.(1)
C(5)	-	C(6)	-	C(22)	119.(1)
N(1)	-	C(8)	-	C(2)	111.(1)
N(1)	-	C(9)	-	C(10)	113.(1)
N(2)	-	C(10)	-	C(9)	118.(1)
N(2)	-	C(10)	-	C(11)	123.(1)

C(9)	-	C(10)	-	C(11)	118.(1)
C(10)	-	C(11)	-	C(12)	118.(1)
C(11)	-	C(12)	-	C(13)	119.(1)
C(12)	-	C(13)	-	C(14)	120.(1)
N(2)	-	C(14)	-	C(13)	121.(1)
N(1)	-	C(15)	-	C(16)	115.(1)
C(15)	-	C(16)	-	C(17)	116.(1)
C(15)	-	C(16)	-	C(21)	125.(1)
C(17)	-	C(16)	-	C(21)	120.(1)
C(16)	-	C(17)	-	C(18)	121.(1)
C(17)	-	C(18)	-	C(19)	119.(1)
C(18)	-	C(19)	-	C(20)	121.(1)
C(19)	-	C(20)	-	C(21)	120.(1)
O(2)	-	C(21)	-	C(16)	123.(1)
O(2)	-	C(21)	-	C(20)	118.(1)
C(16)	-	C(21)	-	C(20)	118.(1)
N(3)	-	C(22)	-	C(6)	112.(1)
N(3)	-	C(23)	-	C(24)	111.(1)
N(4)	-	C(24)	-	C(23)	113.(1)
N(4)	-	C(24)	-	C(25)	126.(1)
C(23)	-	C(24)	-	C(25)	121.(1)
C(24)	-	C(25)	-	C(26)	118.(1)
C(25)	-	C(26)	-	C(27)	118.(1)
C(26)	-	C(27)	-	C(28)	121.(1)

N(4)	-	C(28)	-	C(27)	122.(1)
N(3)	-	C(29)	-	C(30)	116.(1)
C(29)	-	C(30)	-	C(31)	115.(1)
C(29)	-	C(30)	-	C(35)	124.(1)
C(31)	-	C(30)	-	C(35)	121.(1)
C(30)	-	C(31)	-	C(32)	120.(1)
C(31)	-	C(32)	-	C(33)	118.(1)
C(32)	-	C(33)	-	C(34)	123.(1)
C(33)	-	C(34)	-	C(35)	118.(1)
O(3)	-	C(35)	-	C(30)	124.(1)
O(3)	-	C(35)	-	C(34)	116.(1)
C(30)	-	C(35)	-	C(34)	119.(1)
O(4)	-	C(36)	-	O(5)	123.(1)
O(4)	-	C(36)	-	C(37)	118.(1)
O(5)	-	C(36)	-	C(37)	119.(1)
O(6)	-	C(38)	-	O(7)	122.(1)
O(6)	-	C(38)	-	C(39)	119.(1)
O(7)	-	C(38)	-	C(39)	119.(1)
O(8)	-	Cl	-	O(9)	108.(1)
O(8)	-	Cl	-	O(10)	114.(1)
O(8)	-	Cl	-	O(11)	109.(1)
O(9)	-	Cl	-	O(10)	110.(1)
O(9)	-	Cl	-	O(11)	110.(1)
O(10)	-	Cl	-	O(11)	105.(1)

O(8)'	-	Cl	-	O(9)'	105.(1)
O(8)'	-	Cl	-	O(10)'	94.(1)
O(8)'	-	Cl	-	O(11)'	109.(1)
O(9)'	-	Cl	-	O(10)'	110.(1)
O(9)'	-	Cl	-	O(11)'	130.(1)
O(10)'	-	Cl	-	O(11)'	104.(1)

Table VIII. Anisotropic Temperature Factors for [Fe₂ (BBPMP)(OAC)₂] [ClO₄]H₂O

Atom	U(1,1)	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Fe(1)	0.053(1)	0.054(1)	0.048(1)	0.001(1)	0.002(1)	0.003(1)
Fe(2)	0.055(1)	0.049(1)	0.055(1)	0.003(1)	0.006(1)	0.001(1)
O(1)	0.036(3)	0.041(3)	0.027(3)	0.002(3)	-0.005(3)	0.007(3)
O(2)	0.044(3)	0.053(3)	0.044(3)	-0.007(3)	0.003(3)	0.006(3)
O(3)	0.052(3)	0.048(3)	0.042(3)	-0.001(3)	0.003(3)	-0.005(3)
O(4)	0.052(3)	0.064(3)	0.042(3)	-0.009(3)	0.004(3)	0.009(3)
O(5)	0.051(3)	0.064(3)	0.037(3)	0.011(3)	0.009(3)	-0.008(3)
O(6)	0.058(3)	0.045(3)	0.061(3)	0.000(3)	0.024(3)	0.004(3)
O(7)	0.057(3)	0.050(3)	0.054(3)	0.006(3)	0.029(3)	0.011(3)
N(1)	0.040(3)	0.039(3)	0.038(3)	-0.008(3)	-0.002(3)	0.004(3)

N(2)	0.042(3)	0.046(3)	0.046(3)	0.008(3)	0.013(3)	0.012(3)
N(3)	0.033(3)	0.048(3)	0.044(3)	-0.001(3)	-0.002(3)	-0.002(3)
N(4)	0.032(3)	0.047(3)	0.053(3)	-0.004(3)	0.013(3)	-0.012(3)
C(1)	0.023(3)	0.039(3)	0.036(3)	-0.001(3)	0.007(3)	-0.001(3)
C(2)	0.045(3)	0.049(3)	0.046(3)	0.005(3)	0.004(3)	0.010(3)
C(3)	0.053(3)	0.059(3)	0.057(3)	-0.004(3)	0.001(3)	-0.009(3)
C(4)	0.045(3)	0.053(3)	0.062(3)	0.023(3)	-0.013(3)	0.015(3)
C(5)	0.042(3)	0.053(3)	0.056(3)	-0.006(3)	0.012(3)	-0.006(3)
C(6)	0.034(3)	0.043(3)	0.047(3)	0.008(3)	-0.004(3)	-0.007(3)
C(7)	0.079(3)	0.082(3)	0.084(3)	0.005(3)	-0.009(3)	0.013(3)
C(8)	0.043(3)	0.046(3)	0.051(3)	0.000(3)	-0.010(3)	-0.007(3)
C(9)	0.058(3)	0.050(3)	0.046(3)	0.014(3)	0.013(3)	0.002(3)
C(10)	0.038(3)	0.032(3)	0.048(3)	0.007(3)	0.009(3)	-0.004(3)
C(11)	0.056(3)	0.060(3)	0.057(3)	0.010(3)	-0.001(3)	-0.002(3)
C(12)	0.068(3)	0.052(3)	0.074(3)	-0.005(3)	0.009(3)	0.007(3)
C(13)	0.057(3)	0.055(3)	0.060(3)	-0.017(3)	-0.003(3)	-0.002(3)
C(14)	0.065(3)	0.049(3)	0.050(3)	-0.001(3)	0.000(3)	-0.001(3)
C(15)	0.052(3)	0.044(3)	0.044(3)	-0.005(3)	0.006(3)	0.001(3)
C(16)	0.048(3)	0.036(3)	0.043(3)	-0.004(3)	0.009(3)	0.006(3)
C(17)	0.066(3)	0.067(3)	0.058(3)	-0.007(3)	-0.007(3)	0.005(3)
C(18)	0.063(3)	0.066(3)	0.065(3)	-0.006(3)	0.013(3)	0.016(3)
C(19)	0.054(3)	0.060(3)	0.061(3)	0.007(3)	0.005(3)	0.005(3)
C(20)	0.050(3)	0.051(3)	0.043(3)	0.001(3)	-0.004(3)	0.006(3)
C(21)	0.044(3)	0.055(3)	0.054(3)	0.005(3)	-0.003(3)	-0.005(3)

C(22)	0.042(3)	0.037(3)	0.049(3)	0.004(3)	-0.001(3)	0.005(3)
C(23)	0.050(3)	0.052(3)	0.048(3)	0.003(3)	0.002(3)	0.000(3)
C(24)	0.044(3)	0.050(3)	0.045(3)	0.003(3)	0.003(3)	0.002(3)
C(25)	0.059(3)	0.066(3)	0.071(3)	-0.006(3)	0.006(3)	-0.002(3)
C(26)	0.075(3)	0.082(3)	0.076(3)	0.004(3)	-0.002(3)	-0.011(3)
C(27)	0.062(3)	0.058(3)	0.064(3)	-0.013(3)	-0.002(3)	-0.016(3)
C(28)	0.062(3)	0.065(3)	0.067(3)	-0.001(3)	0.008(3)	-0.002(3)
C(29)	0.045(3)	0.039(3)	0.051(3)	0.002(3)	-0.001(3)	0.003(3)
C(30)	0.045(3)	0.048(3)	0.041(3)	-0.003(3)	0.007(3)	-0.002(3)
C(31)	0.065(3)	0.068(3)	0.057(3)	0.007(3)	0.002(3)	-0.001(3)
C(32)	0.075(3)	0.076(3)	0.064(3)	-0.012(3)	0.008(3)	0.005(3)
C(33)	0.065(3)	0.064(3)	0.054(3)	0.017(3)	0.004(3)	-0.009(3)
C(34)	0.048(3)	0.053(3)	0.046(3)	0.004(3)	0.005(3)	0.002(3)
C(35)	0.047(3)	0.068(3)	0.051(3)	0.000(3)	-0.001(3)	-0.007(3)
C(36)	0.034(3)	0.029(3)	0.030(3)	-0.002(3)	-0.010(3)	0.003(3)
C(37)	0.063(3)	0.060(3)	0.049(3)	-0.013(3)	-0.006(3)	-0.003(3)
C(38)	0.052(3)	0.048(3)	0.042(3)	-0.004(3)	0.007(3)	-0.001(3)
C(39)	0.057(3)	0.047(3)	0.060(3)	0.005(3)	0.000(3)	-0.003(3)

Table IX Hydrogen atoms positional parameters for $[\text{Fe}_2(\text{BBPMP})(\text{OAC})_2]$ $[\text{ClO}_4] \cdot \text{H}_2\text{O}$

atom	x	y	z	$B_{\text{eq.}}^a$ ($\text{\AA}^2$)
H3	0.6133	0.2515	0.4602	3.95
H5	0.6598	0.0524	0.2955	3.95
H7	0.7094	0.0978	0.4693	3.95
H7'	0.7673	0.0645	0.3988	3.95
H7''	0.6704	-0.0090	0.4200	3.95
H8	0.5267	0.4063	0.4507	3.95
H8'	0.5271	0.4719	0.3756	3.95
H9	0.3121	0.2964	0.4491	3.95
H9'	0.4265	0.2688	0.4657	3.95
H11	0.4221	0.0739	0.4584	3.95
H12	0.4011	-0.0845	0.3844	3.95
H13	0.3588	-0.0471	0.2697	3.95
H14	0.3109	0.1335	0.2398	3.95
H15	0.3918	0.4838	0.4785	3.95
H15'	0.3928	0.5569	0.4059	3.95
H17	0.2707	0.5681	0.5220	3.95
H18	0.1058	0.5926	0.5288	3.95
H19	0.0064	0.5293	0.4403	3.95

H20	0.0718	0.4415	0.3450	3.95
H22	0.4912	0.1555	0.1980	3.95
H22'	0.5975	0.0922	0.1950	3.95
H23	0.7263	0.1991	0.1900	3.95
H23'	0.7235	0.3102	0.1367	3.95
H25	0.8317	0.2775	0.2683	3.95
H26	0.8455	0.4026	0.3625	3.95
H27	0.7318	0.5508	0.3682	3.95
H28	0.6103	0.5674	0.2925	3.95
H29	0.6140	0.1451	0.0945	3.95
H29'	0.5062	0.2047	0.0974	3.95
H31	0.6398	0.1674	-0.0110	3.95
H32	0.6732	0.2848	-0.1039	3.95
H33	0.6567	0.4842	-0.0951	3.95
H34	0.6067	0.5662	0.0066	3.95
H37	0.3060	0.2749	0.0608	3.95
H37'	0.2174	0.3351	0.1034	3.95
H37''	0.2521	0.2016	0.1218	3.95
H39	0.4475	0.7480	0.2110	3.95
H39'	0.4095	0.7427	0.2905	3.95
H39''	0.3329	0.7233	0.2262	3.95
