Electronic Supplementary Material (ESI) for CrystEngComm.
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Electronic Supplementary Information (ESI) for

Mixed-Solvent/Metal/pH/-Dependent Structural Variations Based on C2-Symmetric 2,6-Bis(3,5-dicarboxylphenyl)pyridine Ligand: Solvothermal Syntheses, Structural Characterizations, and Magnetic Properties

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ESI

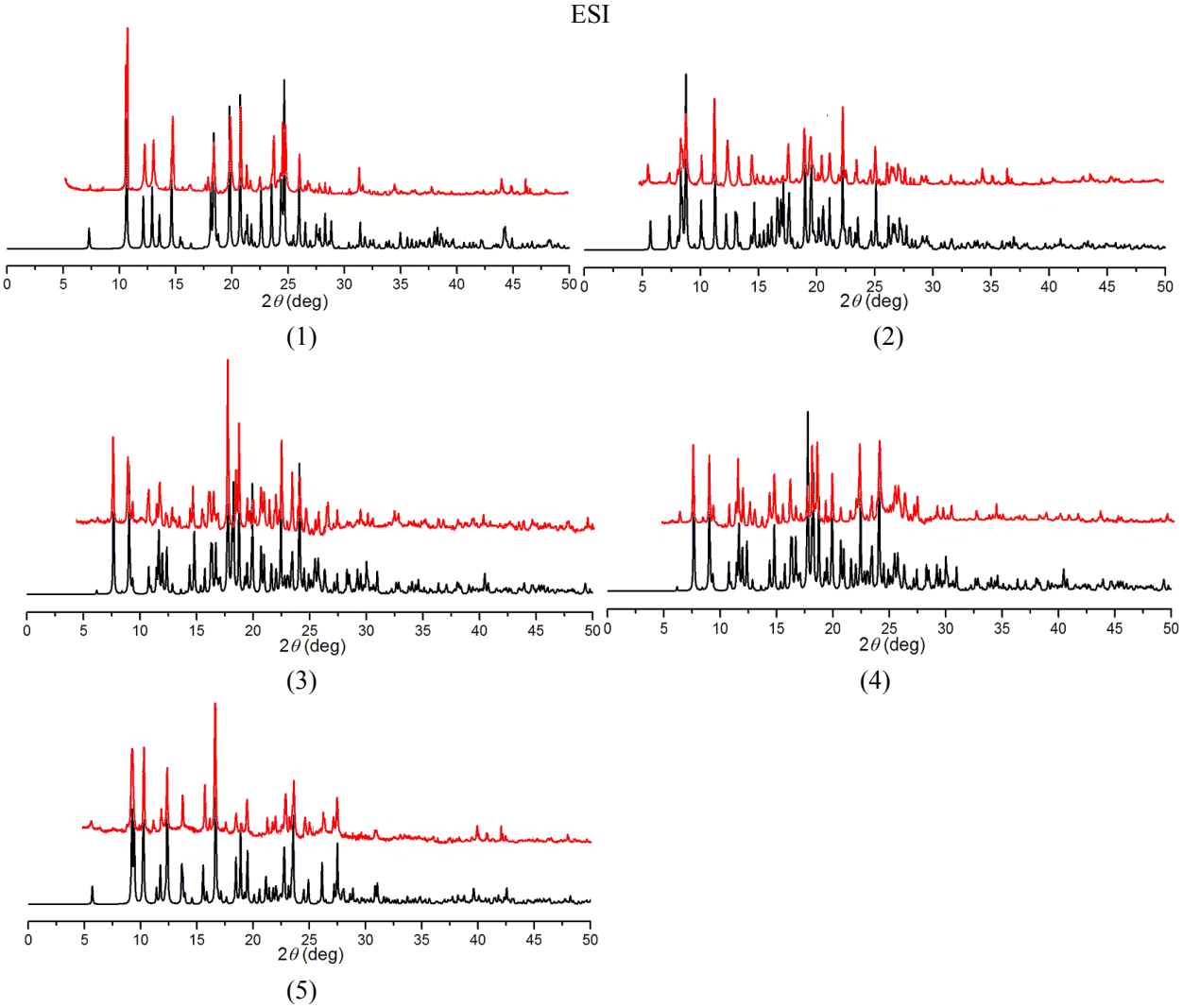
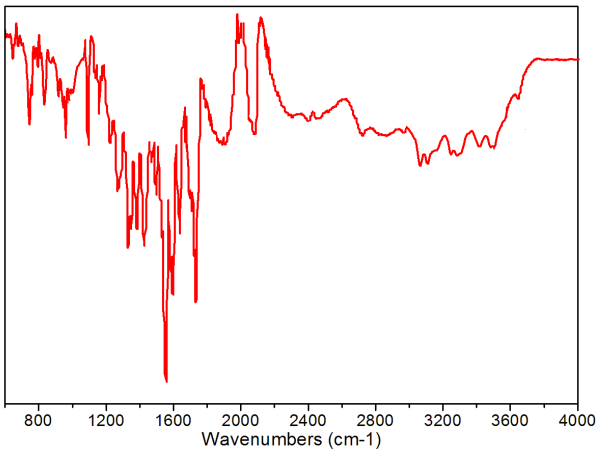


Figure S1. PXRD patterns of **1**-**5**. Dark: calculated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.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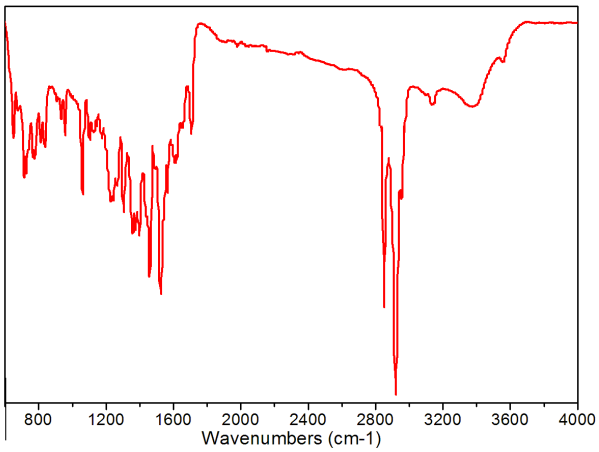
Wavenumbers (cm-1)

(1)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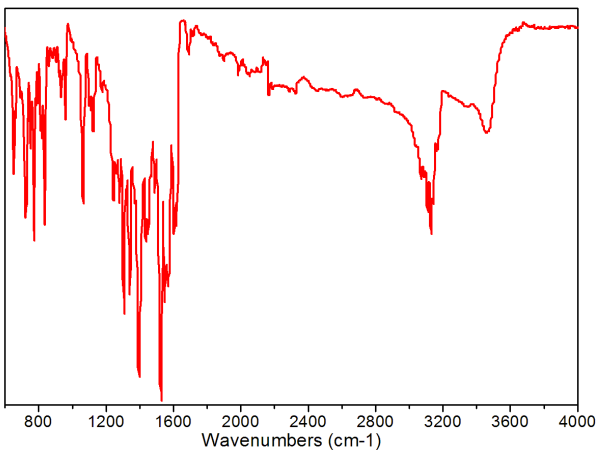
Wavenumbers (cm-1)

(2)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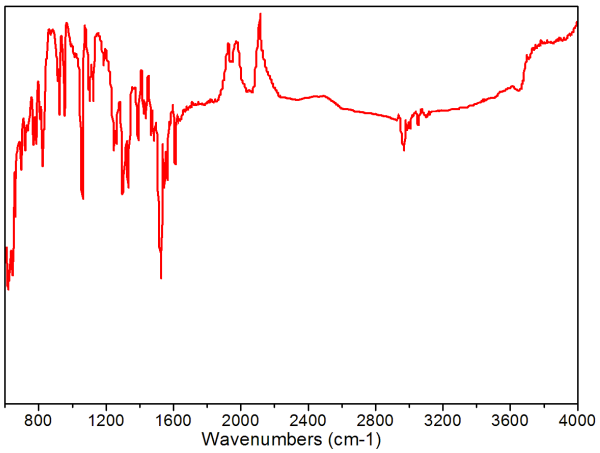
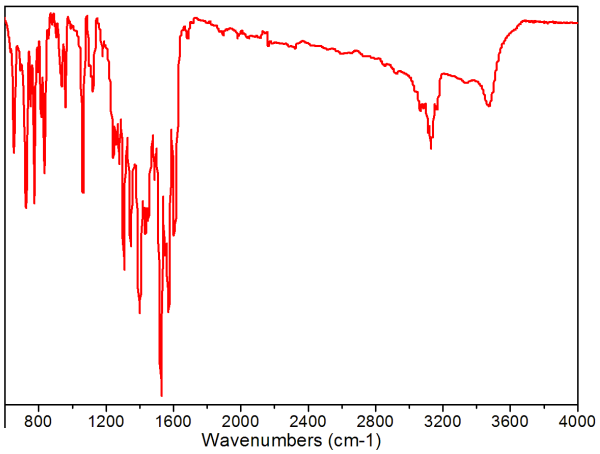
(3)



(4)



(5)

Figure S2. The IR spectras of complexes **1**-**5**.

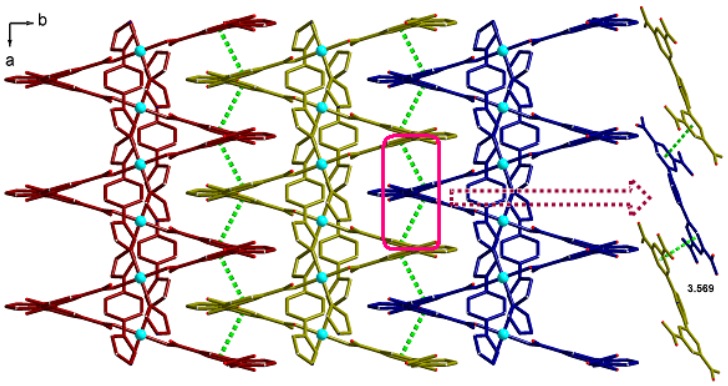


Figure S3. The 3D packing supramolecule structure in **1** view along *c* axis.

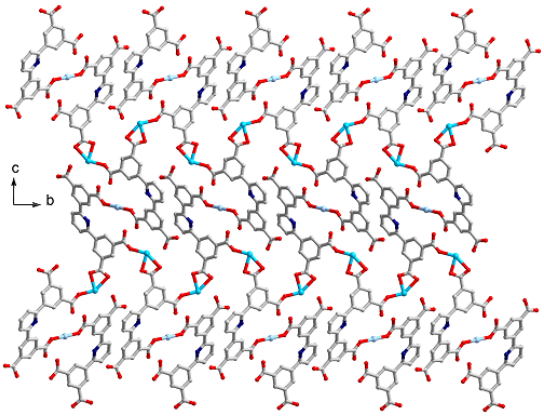


Figure S4. The 2D $[Co_3(HBDP)_2]$ sheet in **2** view along *a* axis.

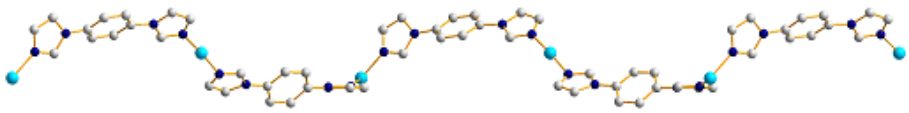


Figure S5. The 1D [Co(bib)] helix chain in **3**.

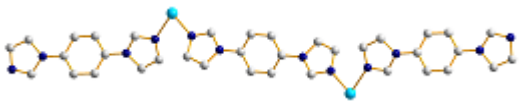


Figure S6. The $Mn_2(bib)_3$ trimer in **4**.

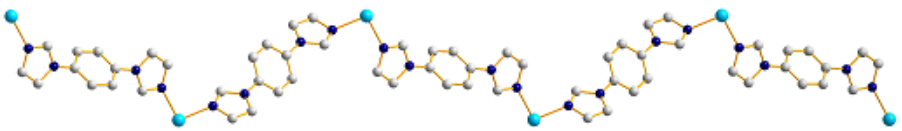
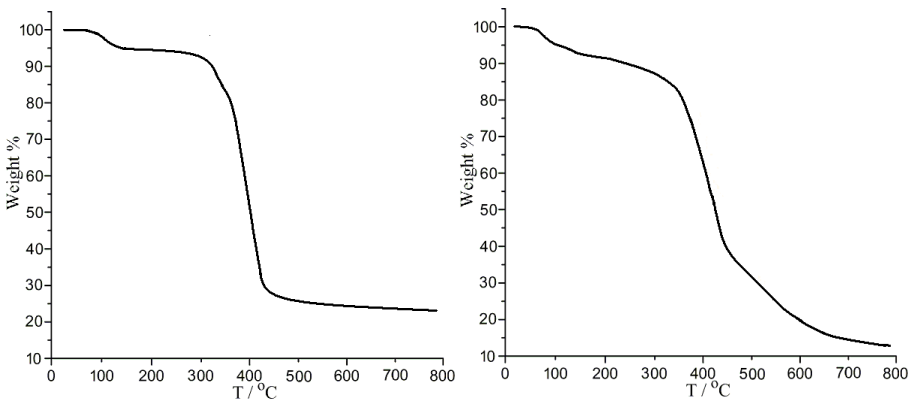


Figure S7. The 1D [Fe(bib)] zigzag chain in **5**.



(1) (2)

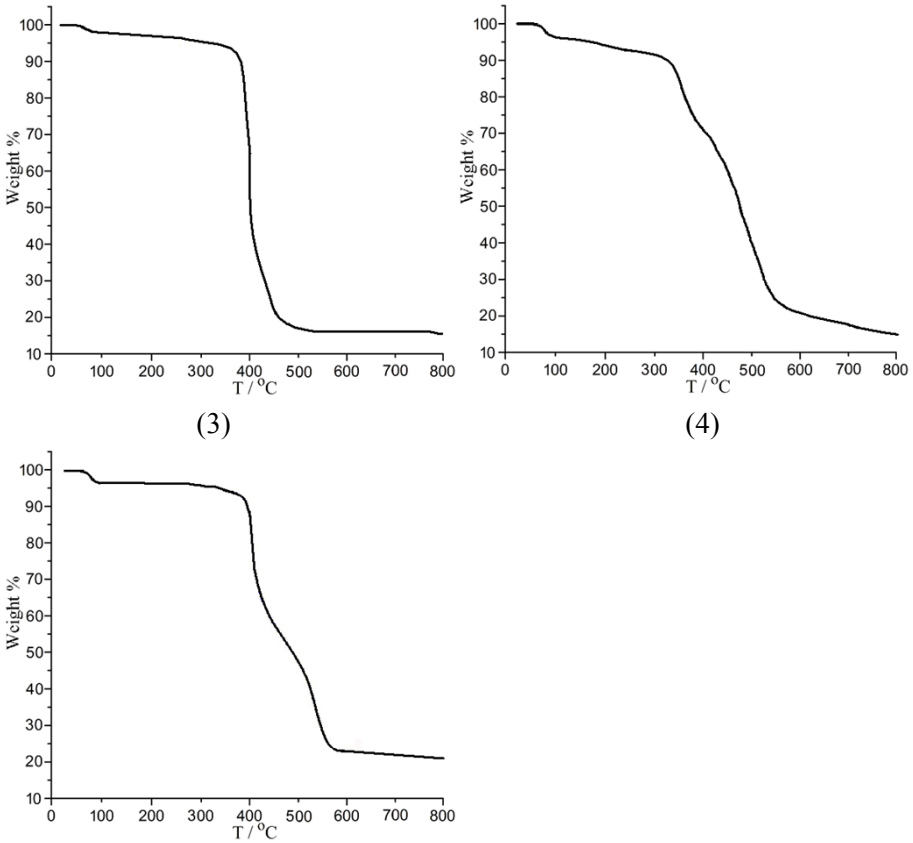


Figure S8. TG curves of **1**-**5**.

Table S1 Selected bond lengths (Å) and angles (º) for **1 – 5**.

Complex **1**							
Cu(1)-N(2)$^{\#3}$	1.973(3)	Cu(1)-N(2)	1.973(3)	Cu(1)-O(3)$^{\#3}$	1.979(3)	Cu(1)-O(3)	1.979(3)
N(2)$^{\#3}$-Cu(1)-N(2)	180.00(18)	N(2)-Cu(1)-O(3)$^{\#3}$	91.72(13)	N(2)-Cu(1)-O(3)	88.28(13)	O(3)$^{\#3}$-Cu(1)-O(3)	180.0(17)
N(2)$^{\#3}$-Cu(1)-O(3)$^{\#3}$	88.28(13)	N(2)$^{\#3}$-Cu(1)-O(3)	91.72(13)				
Symmetry code: #3 -*x*+1, -*y*+2, -*z*.							
Complex **2**							
Co(1)-O(1)	2.019(3)	Co(1)-N(2)	2.131(3)	Co(2)-O(5)	2.072(3)	Co(2)-N(8)	2.139(3)
Co(1)-N(6)$^{\#3}$	2.107(3)	Co(1)-O(3)$^{\#4}$	2.178(3)	Co(2)-O(5)$^{\#5}$	2.072(3)	Co(2)-O(1W)	2.172(3)
Co(1)-N(4)	2.110(3)	Co(1)-O(4)$^{\#4}$	2.286(3)	Co(2)-N(8)$^{\#5}$	2.139(3)	Co(2)-O(1W)$^{\#5}$	2.172(3)
O(1)-Co(1)-N(6)$^{\#3}$	92.59(12)	N(4)-Co(1)-O(3)$^{\#4}$	157.71(13)	O(5)-Co(2)-N(8)$^{\#5}$	91.29(12)	N(8)$^{\#5}$-Co(2)-O(1W)	92.11(11)
O(1)-Co(1)-N(4)	113.66(12)	N(2)-Co(1)-O(3)$^{\#4}$	89.29(11)	O(5)$^{\#5}$-Co(2)-N(8)$^{\#5}$	88.71(12)	N(8)-Co(2)-O(1W)	87.89(11)
N(6)-Co(1)-N(4)	87.32(12)	O(1)-Co(1)-O(4)$^{\#4}$	146.71(10)	O(5)-Co(2)-N(8)	88.71(12)	O(5)-Co(2)-O(1W)$^{\#5}$	89.64(11)
O(1)-Co(1)-N(2)	92.01(12)	N(6)$^{\#3}$-Co(1)-O(4)$^{\#4}$	91.93(11)	O(5)$^{\#5}$-Co(2)-N(8)	91.29(12)	O(5)$^{\#5}$-Co(2)-O(1W)$^{\#5}$	90.36(11)
N(6)-Co(1)-N(2)	174.72(12)	N(4)-Co(1)-O(4)$^{\#4}$	99.48(12)	N(8)$^{\#5}$-Co(2)-N(8)	180.00(17)	N(8)$^{\#5}$-Co(2)-O(1W)$^{\#5}$	87.89(11)
N(4)-Co(1)-N(2)	93.22(12)	N(2)-Co(1)-O(4)$^{\#4}$	82.80(11)	O(5)-Co(2)-O(1W)	90.36(11)	N(8)-Co(2)-O(1W)$^{\#5}$	92.11(11)
O(1)-Co(1)-O(3)$^{\#4}$	88.35(11)	O(3)$^{\#4}$-Co(1)-O(4)$^{\#4}$	58.84(10)	O(5)$^{\#5}$-Co(2)-O(1W)	89.64(11)	O(1W)-Co(2)-O(1W)$^{\#5}$	180.000(1)
N(6)$^{\#3}$-Co(1)-O(3)$^{\#4}$	88.24(11)	O(5)-Co(2)-O(5)$^{\#5}$	180.00(14)				
Symmetry codes: #3 *x*+1/2, *y*+1/2, *z*; #4 -*x*+1/2, *y*-1/2, -*z*+1/2; #5 -*x*+1, -*y*+1,-*z*+1; #6 -*x*+1/2, *y*+1/2, -*z*+1/2.							
Complex **3**							
Co(1)-O(4)$^{\#2}$	2.031(3)	Co(1)-N(8)$^{\#1}$	2.111(3)	Co(2)-O(1)	1.977(2)	Co(2)-O(6)$^{\#5}$	2.063(3)
Co(1)-N(7)$^{\#3}$	2.107(3)	Co(1)-O(8)$^{\#4}$	2.225(3)	Co(2)-N(4)	2.049(3)	Co(2)-O(5)$^{\#5}$	2.315(2)
Co(1)-O(3)	2.110(2)	Co(1)-O(7)$^{\#4}$	2.266(3)	Co(2)-N(2)	2.057(3)	O(1)-Co(2)-O(6)$^{\#5}$	105.26(10)
O(4)$^{\#2}$-Co(1)-N(7)$^{\#3}$	92.45(12)	O(4)$^{\#2}$-Co(1)-O(8)$^{\#4}$	89.16(11)	O(3)-Co(1)-O(7)$^{\#4}$	87.61(9)	N(4)-Co(2)-O(6)$^{\#5}$	126.81(12)
O(4)$^{\#2}$-Co(1)-O(3)	125.51(10)	N(7)$^{\#3}$-Co(1)-O(8)$^{\#4}$	85.96(11)	N(40)$^{\#1}$-Co(1)-O(7)$^{\#4}$	96.03(11)	N(2)-Co(2)-O(6)$^{\#5}$	114.33(11)
N(7)$^{\#3}$-Co(1)-O(3)	90.21(11)	O(3)-Co(1)-O(8)$^{\#4}$	145.28(10)	O(8)$^{\#4}$-Co(1)-O(7)$^{\#4}$	57.76(10)	O(1)-Co(2)-O(5)$^{\#5}$	160.68(11)
O(4)$^{\#2}$-Co(1)-N(8)$^{\#1}$	86.64(11)	N(40)$^{\#1}$-Co(1)-O(8)$^{\#4}$	98.70(11)	O(1)-Co(2)-N(4)	93.96(11)	N(4)-Co(2)-O(5)$^{\#5}$	88.20(10)
N(7)$^{\#3}$-Co(1)-N(8)$^{\#1}$	175.23(12)	O(4)$^{\#2}$-Co(1)-O(7)$^{\#4}$	146.88(11)	O(1)-Co(2)-N(2)	114.39(11)	N(2)-Co(2)-O(5)$^{\#5}$	83.92(10)
O(3)-Co(1)-N(8)$^{\#1}$	86.53(10)	N(7)$^{\#3}$-Co(1)-O(7)$^{\#4}$	87.30(11)	N(4)-Co(2)-N(2)	100.82(12)	O(6)$^{\#5}$-Co(2)-O(5)$^{\#5}$	59.14(9)
Symmetry codes: #1 -*x*+1/2, *y*+1/2, -*z*+3/2; #2 -*x*-1, -*y*+2, -*z*+1; #3 -*x*-1, -*y*+1, -*z*+1; #4 *x*-1, *y*-1, *z*; #5 -*x*+1/2, *y*-1/2, -*z*+3/2.							
Complex **4**							
Mn(1)-O(4)	2.1428(15)	Mn(1)-O(2)$^{\#3}$	2.1631(15)	Mn(1)-N(5)	2.2481(19)	Mn(1)-O(6)	2.3303(9)
Mn(1)-O(7)	2.1514(16)	Mn(1)-N(4)	2.232(2)	O(7)-Mn(1)-N(5)	91.01(7)	O(7)-Mn(1)-O(6)	84.49(6)
O(4)-Mn(1)-O(7)	171.57(6)	O(7)-Mn(1)-N(4)	88.73(7)	O(2)$^{\#3}$-Mn(1)-N(5)	174.51(7)	O(2)$^{\#3}$-Mn(1)-O(6)	85.48(5)
O(4)-Mn(1)-O(2)$^{\#3}$	90.51(6)	O(2)$^{\#3}$-Mn(1)-N(4)	92.53(7)	N(4)-Mn(1)-N(5)	92.83(7)	N(4)-Mn(1)-O(6)	173.00(7)
O(7)-Mn(1)-O(2)$^{\#3}$	87.97(7)	O(4)-Mn(1)-N(5)	89.72(7)	O(4)-Mn(1)-O(6)	87.12(6)	N(5)-Mn(1)-O(6)	89.06(6)
O(4)-Mn(1)-N(4)	99.62(7)						
Symmetry code: #3 -*x*+1/2, *y*+1/2, -*z*+1/2.							
Complex **5**							
Fe(1)-N(4)	2.104(2)	Fe(1)-O(4)$^{\#4}$	2.1922(17)	Fe(2)-O(1)	2.0763(16)	Fe(2)-O(8)$^{\#5}$	2.1530(18)
Fe(1)-O(6)$^{\#3}$	2.1335(18)	Fe(1)-O(1)	2.2468(17)	Fe(2)-O(5)$^{\#3}$	2.0991(17)	Fe(2)-O(4)$^{\#4}$	2.1883(17)
Fe(1)-N(1)	2.169(2)	Fe(1)-O(2)	2.3684(18)	Fe(2)-O(1W)	2.130(2)	Fe(2)-O(7)$^{\#5}$	2.2717(19)
N(4)-Fe(1)-O(6)$^{\#3}$	84.74(8)	N(1)-Fe(1)-O(1)	89.29(7)	O(1)-Fe(2)-O(1W)	88.42(8)	O(1W)-Fe(2)-O(4)$^{\#4}$	164.69(8)
N(4)-Fe(1)-N(1)	96.59(8)	O(4)$^{\#4}$-Fe(1)-O(1)	72.94(6)	O(5)$^{\#3}$-Fe(2)-O(1W)	95.20(9)	O(8)$^{\#5}$-Fe(2)-O(4)$^{\#4}$	106.93(7)
O(6)$^{\#3}$-Fe(1)-N(1)	177.26(8)	N(4)-Fe(1)-O(2)	89.41(7)	O(1)-Fe(2)-O(8)$^{\#5}$	153.36(7)	O(1)-Fe(2)-O(7)$^{\#5}$	94.62(7)
N(4)-Fe(1)-O(4)$^{\#4}$	140.40(7)	O(6)$^{\#3}$-Fe(1)-O(2)	91.77(7)	O(5)$^{\#3}$-Fe(2)-O(8)$^{\#5}$	94.16(7)	O(5)$^{\#3}$-Fe(2)-O(7)$^{\#5}$	152.78(7)
O(6)$^{\#3}$-Fe(1)-O(4)$^{\#4}$	86.61(7)	N(1)-Fe(1)-O(2)	85.86(8)	O(1W)-Fe(2)-O(8)$^{\#5}$	87.57(9)	O(1W)-Fe(2)-O(7)$^{\#5}$	88.20(10)
N(1)-Fe(1)-O(4)$^{\#4}$	93.83(7)	O(4)$^{\#4}$-Fe(1)-O(2)	129.48(6)	O(1)-Fe(2)-O(4)$^{\#4}$	76.41(6)	O(8)$^{\#5}$-Fe(2)-O(7)$^{\#5}$	58.94(7)
N(4)-Fe(1)-O(1)	145.01(7)	O(1)-Fe(1)-O(2)	56.54(6)	O(5)$^{\#3}$-Fe(2)-O(4)$^{\#4}$	88.78(7)	O(4)$^{\#4}$-Fe(2)-O(7)$^{\#5}$	95.02(8)
O(6)$^{\#3}$-Fe(1)-O(1)	88.26(7)	O(1)-Fe(2)-O(5)$^{\#3}$	112.43(7)				
Symmetry codes: #3 -*x*+1, -*y*+1, -*z*+1; #4 *x*-1, *y*, *z*; #5 -*x*+1, -*y*, -*z*+1.							