

**Influence of ionic liquids on the syntheses and structures of Mn(II) coordination  
polymers based on multidentate N-heterocyclic aromatic ligand  
and bridging carboxylate ligands**

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## *Supporting Information*

*1. Supporting Figures.*

*2. PXRD patterns.*

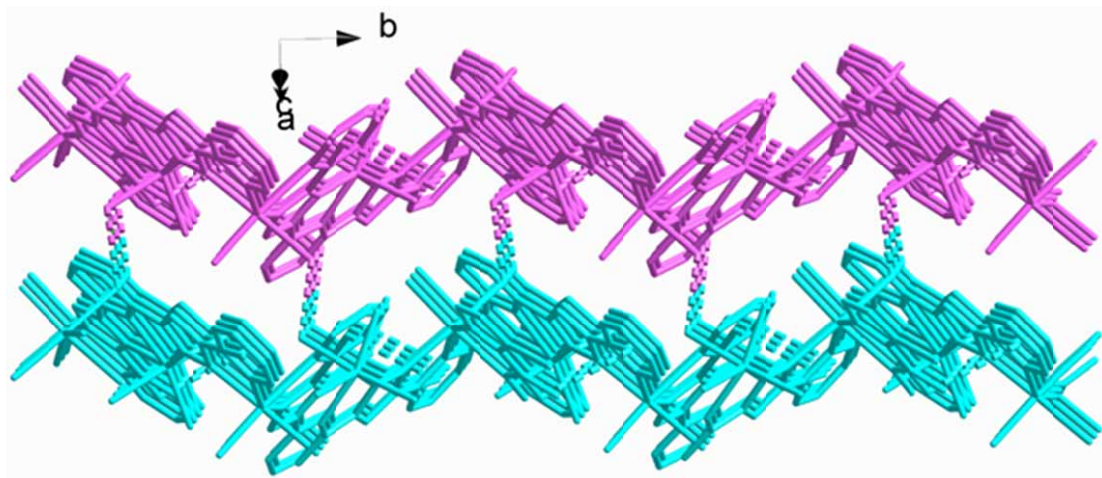
*3. TG curves.*

*4. Table for the Curie-Weiss data and the  $J/g$  values.*

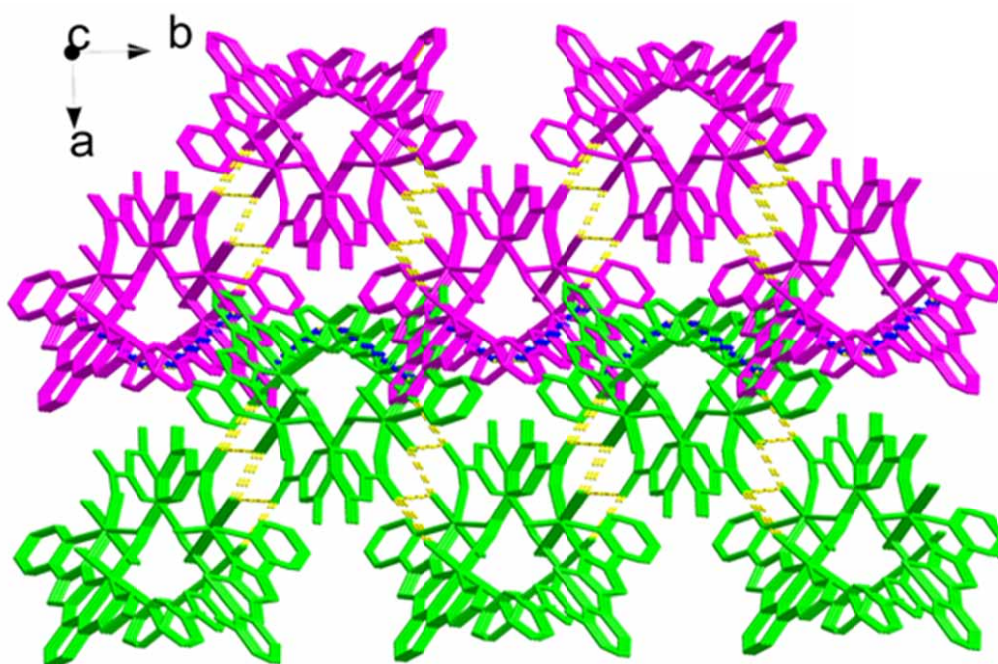
*5. Table for the selected bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ).*

*6. Table for the selected hydrogen bonds.*

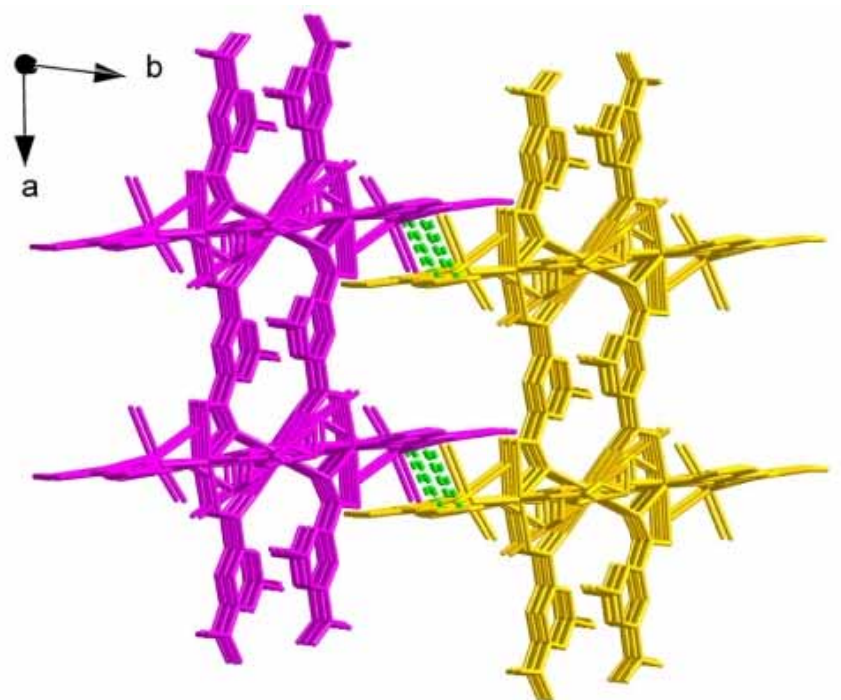
## 1. Supporting Figures.



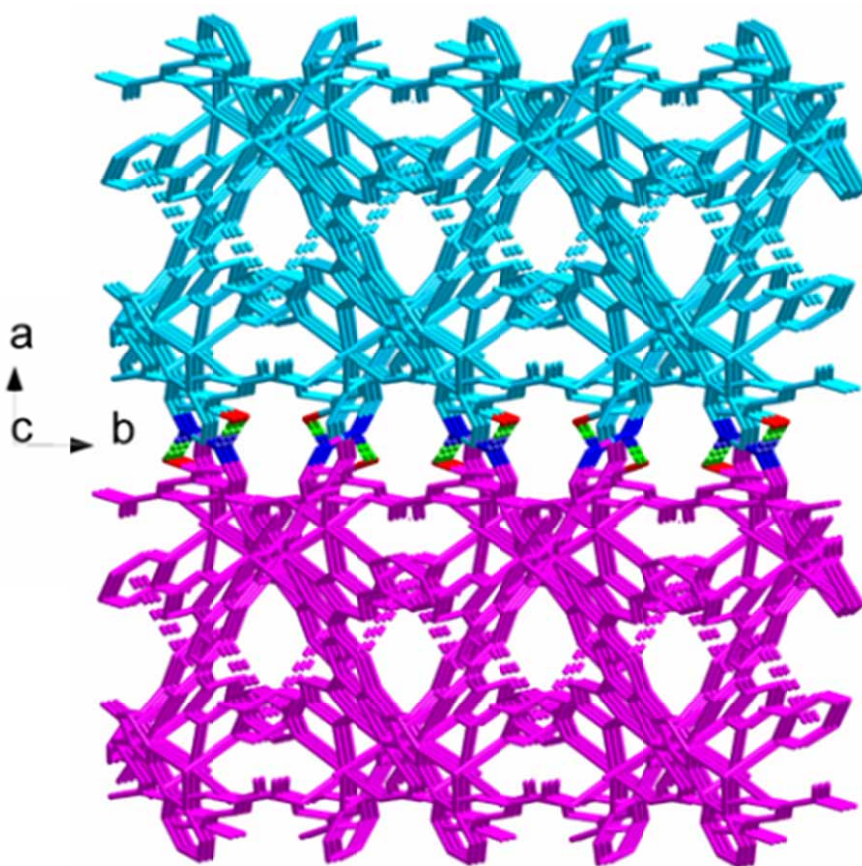
**Fig.S1** View of 3D supramolecular framework in **1**. H atoms are omitted for clarity.



**Fig. S2** View of 3D supramolecular framework in **4**. H atoms are omitted for clarity.

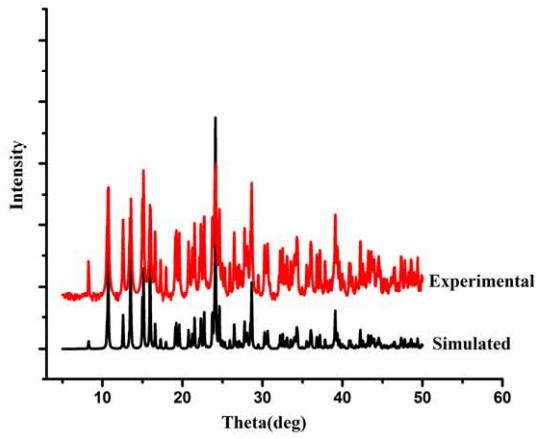


**Fig. S3** View of 3D supramolecular framework in **5**. H atoms are omitted for clarity.

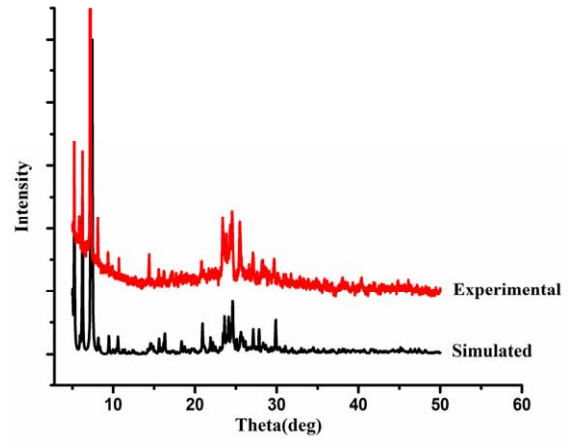


**Fig.S4** View of the final 3D supramolecular framework in **6**. H atoms are omitted for clarity.

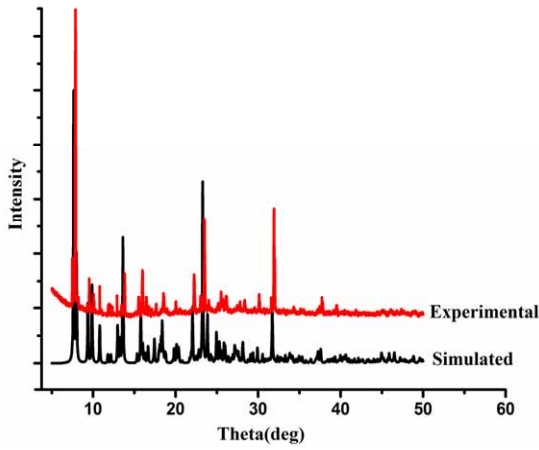
## 2. PXRD patterns.



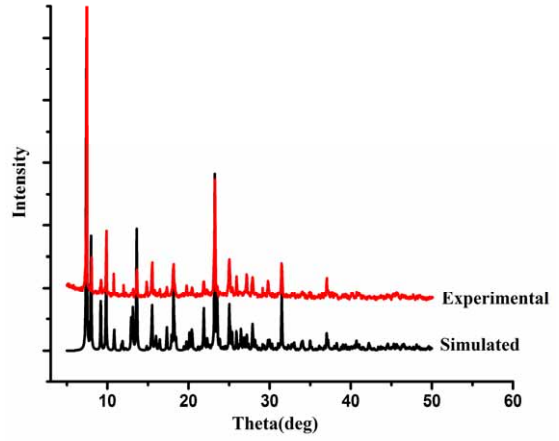
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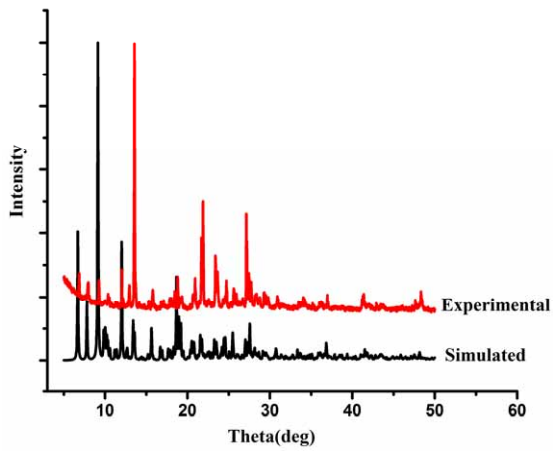
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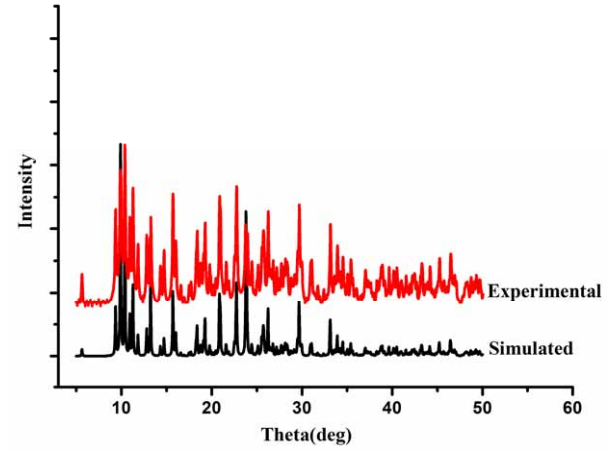
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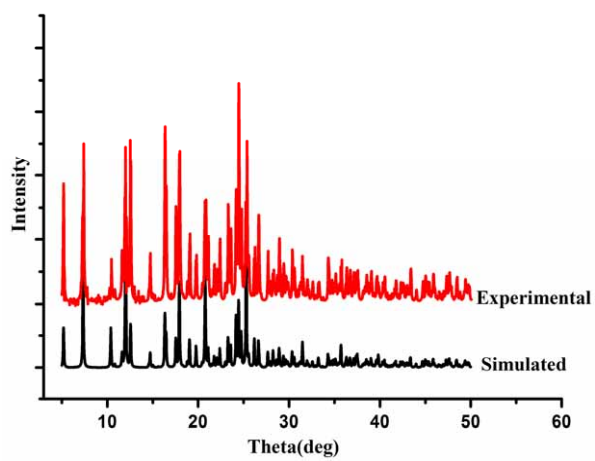
(4)



(5)



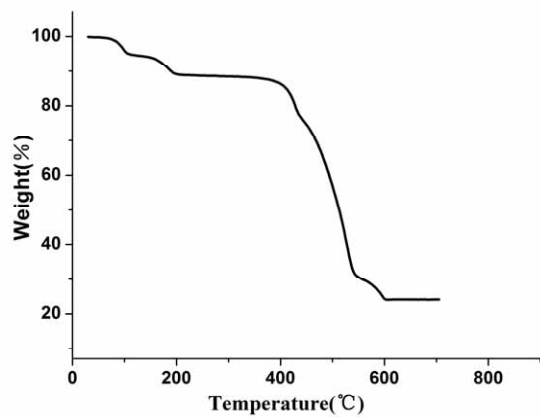
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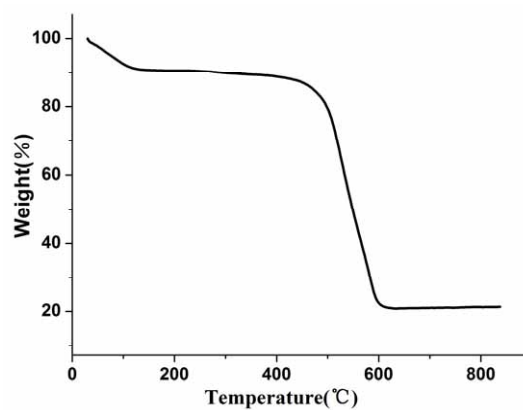
(7)

Fig. S5 Powder X-ray diffraction profiles for complex 1-7.

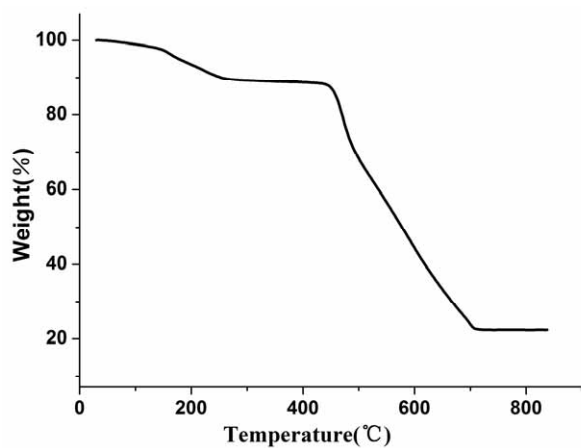
### 3. TG curves.



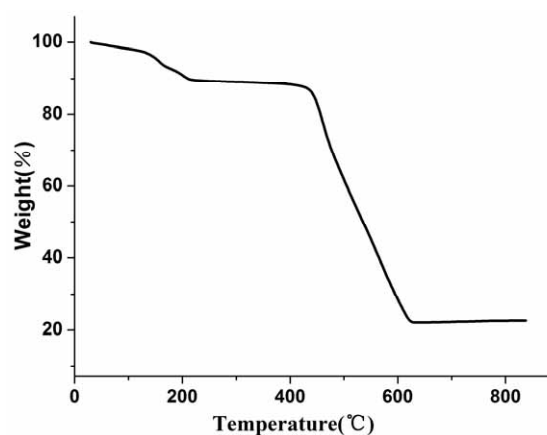
(1)



(2)

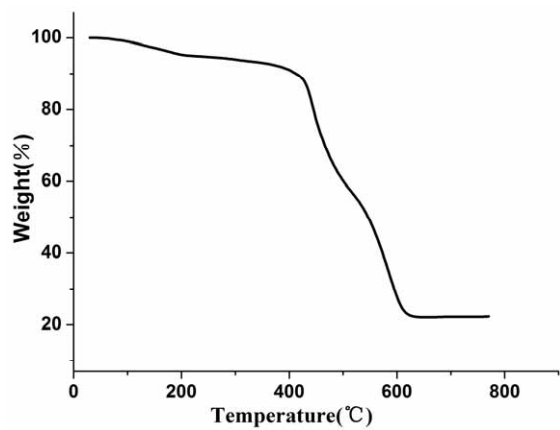


(3)

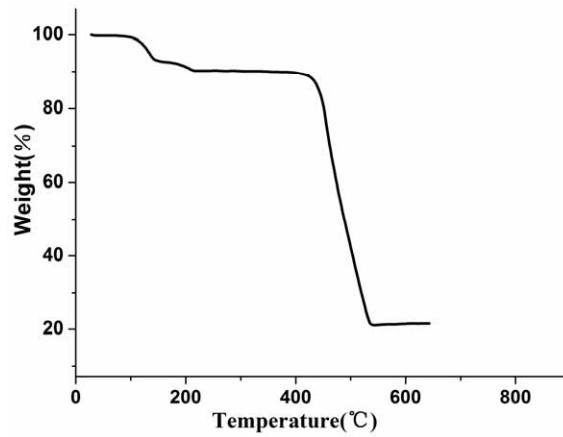


(4)

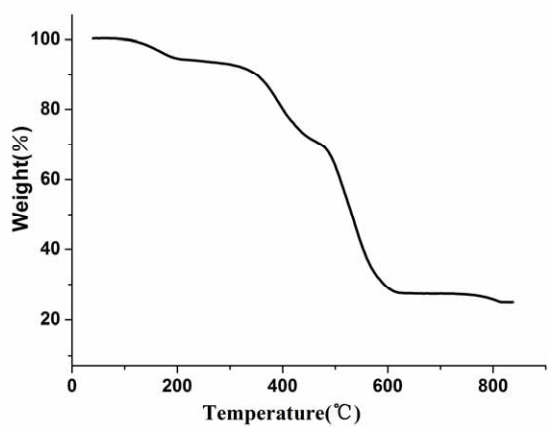




(5)



(6)



(7)

Fig. S6 Thermogravimetric curves of complexes 1–7.

#### 4. Table for the Curie-Weiss data and the $J/g$ values.

**Table S1.** Curie-Weiss data and the  $J/g$  values for complex 1-7.

Complexes	$\theta$ (K)	$C$ (cm <sup>3</sup> K mol <sup>-1</sup> )	$R$	$J$ (cm <sup>-1</sup> )	$g$	$R$
1	-3.4	9.09	$1.78 \times 10^{-4}$	-1.01	1.98	$2.34 \times 10^{-3}$
2	-16.96	33.47	/	/	/	/
3	-6.11	8.79	$1.27 \times 10^{-4}$	-0.54	1.99	$3.19 \times 10^{-4}$
4	-6.20	8.80	$1.28 \times 10^{-4}$	-0.47	1.99	$3.58 \times 10^{-4}$
5	-13.10	14.91	$1.15 \times 10^{-4}$	$J_1 = -1.27$ $J_2 = -1.65$	1.85	$1.16 \times 10^{-4}$
6	-10.90	8.90	$1.75 \times 10^{-4}$	-1.95	2.01	$1.23 \times 10^{-4}$
7	-3.55	8.97	$1.54 \times 10^{-4}$	$J_1 = -0.18$ $J_2 = -0.1$	1.98	$5.9 \times 10^{-4}$

#### 5. Table for selected bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ).

**Table S2.** Selected bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ) for complex 1-7.

Complex 1			
Mn(1)-O(3)	2.151(4)	Mn(2)-O(1)	2.157(3)
Mn(1)-N(4)#1	2.173(3)	Mn(2)-O(2)	2.247(3)
Mn(1)-N(7)	2.266(4)	Mn(2)-N(11)	2.249(3)
Mn(1)-N(9)	2.320(4)	Mn(2)-N(6)	2.323(3)
Mn(1)-N(2)#1	2.439(4)	Mn(2)-N(3)	2.326(3)
Mn(1)-Cl(2)	2.4737(16)		
O(3)-Mn(1)-N(4)#1	109.81(15)	O(1)-Mn(2)-O(2)	80.01(12)
O(3)-Mn(1)-N(7)	88.26(15)	O(1)-Mn(2)-N(11)	158.45(12)
N(4)#1-Mn(1)-N(7)	96.95(13)	O(2)-Mn(2)-N(11)	80.70(13)
O(3)-Mn(1)-N(9)	94.30(15)	O(1)-Mn(2)-N(6)	100.37(12)
N(4)#1-Mn(1)-N(9)	153.97(13)	O(2)-Mn(2)-N(6)	94.54(13)
N(7)-Mn(1)-N(9)	73.46(13)	N(11)-Mn(2)-N(6)	71.69(12)
O(3)-Mn(1)-N(2)#1	174.01(14)	O(1)-Mn(2)-N(3)	114.81(13)



N(4)#1-Mn(1)-N(2)#1	71.85(12)	O(2)-Mn(2)-N(3)	83.35(12)
N(7)-Mn(1)-N(2)#1	97.31(11)	N(11)-Mn(2)-N(3)	72.18(12)
N(9)-Mn(1)-N(2)#1	85.19(12)	N(6)-Mn(2)-N(3)	143.67(12)
O(3)-Mn(1)-Cl(2)	88.54(12)	O(1)-Mn(2)-Cl(1)	93.16(9)
N(4)#1-Mn(1)-Cl(2)	95.19(10)	O(2)-Mn(2)-Cl(1)	166.18(11)
N(7)-Mn(1)-Cl(2)	167.83(10)	N(11)-Mn(2)-Cl(1)	107.67(9)
N(9)-Mn(1)-Cl(2)	95.08(10)	N(6)-Mn(2)-Cl(1)	98.52(10)
N(2)#1-Mn(1)-Cl(2)	85.56(9)	N(3)-Mn(2)-Cl(1)	88.74(9)

Complex 2

Mn(1)-N(36)	2.187(6)	Mn(5)-N(8)	2.149(6)
Mn(1)-N(6)	2.263(6)	Mn(5)-N(39)	2.262(5)
Mn(1)-N(4)	2.286(7)	Mn(5)-N(40)	2.272(5)
Mn(1)-N(7)	2.326(6)	Mn(5)-N(37)	2.290(6)
Mn(1)-N(34)	2.463(8)	Mn(5)-Cl(2)	2.555(2)
Mn(1)-Cl(1)	2.836(2)	Mn(6)-N(30)	2.187(5)
Mn(2)-N(59)	2.198(6)	Mn(6)-N(62)	2.282(5)
Mn(2)-N(28)	2.272(6)	Mn(6)-N(61)	2.283(6)
Mn(2)-N(26)	2.298(6)	Mn(6)-N(58)	2.319(6)
Mn(2)-N(29)	2.343(6)	Mn(6)-N(32)	2.454(6)
Mn(2)-N(56)	2.485(6)	Mn(6)-Cl(2)	2.5355(19)
Mn(2)-Cl(1)	2.5004(19)	Mn(7)-N(3)	2.157(8)
Mn(3)-N(14)	2.167(5)	Mn(7)-N(25)	2.160(7)
Mn(3)-N(48)	2.268(6)	Mn(7)-N(47)	2.194(7)
Mn(3)-N(50)	2.278(6)	Mn(7)-N(23)	2.320(7)
Mn(3)-N(51)	2.309(5)	Mn(7)-N(1)	2.379(7)
Mn(3)-N(12)	2.490(6)	Mn(7)-N(45)	2.501(8)
Mn(3)-Cl(1)	2.522(2)	Mn(8)-N(63)	2.173(6)
Mn(4)-N(52)	2.190(6)	Mn(8)-N(41)	2.183(5)
Mn(4)-N(17)	2.260(6)	Mn(8)-N(19)	2.202(5)
Mn(4)-N(18)	2.286(5)	Mn(8)-N(21)	2.348(6)
Mn(4)-N(15)	2.333(6)	Mn(8)-N(43)	2.405(6)
Mn(4)-N(54)	2.452(6)	Mn(8)-N(65)	2.432(6)
Mn(4)-Cl(2)	2.5321(19)		
N(36)-Mn(1)-N(6)	151.3(2)	N(15)-Mn(4)-Cl(2)	107.73(16)
N(36)-Mn(1)-N(4)	138.0(2)	N(54)-Mn(4)-Cl(2)	118.87(15)

N(6)-Mn(1)-N(4)	70.7(2)	N(8)-Mn(5)-N(39)	138.5(2)
N(36)-Mn(1)-N(7)	84.5(2)	N(8)-Mn(5)-N(40)	134.7(2)
N(6)-Mn(1)-N(7)	68.7(2)	N(39)-Mn(5)-N(40)	72.1(2)
N(4)-Mn(1)-N(7)	134.2(2)	N(8)-Mn(5)-N(37)	83.8(2)
N(36)-Mn(1)-N(34)	70.9(2)	N(39)-Mn(5)-N(37)	70.1(2)
N(6)-Mn(1)-N(34)	125.4(2)	N(40)-Mn(5)-N(37)	140.1(2)
N(4)-Mn(1)-N(34)	80.4(2)	N(8)-Mn(5)-Cl(2)	86.17(17)
N(7)-Mn(1)-N(34)	141.9(2)	N(39)-Mn(5)-Cl(2)	131.20(15)
N(36)-Mn(1)-Cl(1)	77.91(17)	N(40)-Mn(5)-Cl(2)	89.27(15)
N(6)-Mn(1)-Cl(1)	113.89(17)	N(37)-Mn(5)-Cl(2)	106.33(16)
N(4)-Mn(1)-Cl(1)	81.5(2)	N(30)-Mn(6)-N(62)	142.6(2)
N(7)-Mn(1)-Cl(1)	96.26(17)	N(30)-Mn(6)-N(61)	135.0(2)
N(34)-Mn(1)-Cl(1)	105.96(17)	N(62)-Mn(6)-N(61)	70.5(2)
N(59)-Mn(2)-N(28)	126.7(2)	N(30)-Mn(6)-N(58)	81.1(2)
N(59)-Mn(2)-N(26)	143.3(2)	N(62)-Mn(6)-N(58)	135.6(2)
N(28)-Mn(2)-N(26)	71.2(2)	N(61)-Mn(6)-N(58)	69.3(2)
N(59)-Mn(2)-N(29)	78.8(2)	N(30)-Mn(6)-N(32)	70.31(19)
N(28)-Mn(2)-N(29)	68.8(2)	N(62)-Mn(6)-N(32)	78.9(2)
N(26)-Mn(2)-N(29)	135.5(2)	N(61)-Mn(6)-N(32)	101.0(2)
N(59)-Mn(2)-N(56)	69.2(2)	N(58)-Mn(6)-N(32)	126.78(19)
N(28)-Mn(2)-N(56)	92.7(2)	N(30)-Mn(6)-Cl(2)	86.88(15)
N(26)-Mn(2)-N(56)	79.1(2)	N(62)-Mn(6)-Cl(2)	88.82(15)
N(29)-Mn(2)-N(56)	121.2(2)	N(61)-Mn(6)-Cl(2)	132.19(15)
N(59)-Mn(2)-Cl(1)	92.40(15)	N(58)-Mn(6)-Cl(2)	104.65(15)
N(28)-Mn(2)-Cl(1)	136.64(15)	N(32)-Mn(6)-Cl(2)	117.07(14)
N(26)-Mn(2)-Cl(1)	88.60(17)	N(3)-Mn(7)-N(25)	109.3(3)
N(29)-Mn(2)-Cl(1)	107.41(15)	N(3)-Mn(7)-N(47)	110.0(2)
N(56)-Mn(2)-Cl(1)	121.49(15)	N(25)-Mn(7)-N(47)	97.0(2)
N(14)-Mn(3)-N(48)	141.3(2)	N(3)-Mn(7)-N(23)	100.7(3)
N(14)-Mn(3)-N(50)	131.7(2)	N(25)-Mn(7)-N(23)	74.1(2)
N(48)-Mn(3)-N(50)	71.0(2)	N(47)-Mn(7)-N(23)	149.2(3)
N(14)-Mn(3)-N(51)	80.9(2)	N(3)-Mn(7)-N(1)	73.1(3)
N(48)-Mn(3)-N(51)	136.0(2)	N(25)-Mn(7)-N(1)	163.9(2)
N(50)-Mn(3)-N(51)	68.7(2)	N(47)-Mn(7)-N(1)	97.0(2)
N(14)-Mn(3)-N(12)	70.0(2)	N(23)-Mn(7)-N(1)	89.8(2)

N(48)-Mn(3)-N(12)	77.9(2)	N(3)-Mn(7)-N(45)	156.3(3)
N(50)-Mn(3)-N(12)	95.3(2)	N(25)-Mn(7)-N(45)	93.6(3)
N(51)-Mn(3)-N(12)	122.4(2)	N(47)-Mn(7)-N(45)	71.5(2)
N(14)-Mn(3)-Cl(1)	88.40(16)	N(23)-Mn(7)-N(45)	79.5(3)
N(48)-Mn(3)-Cl(1)	89.91(16)	N(1)-Mn(7)-N(45)	83.2(3)
N(50)-Mn(3)-Cl(1)	135.13(15)	N(63)-Mn(8)-N(41)	104.6(2)
N(51)-Mn(3)-Cl(1)	106.55(16)	N(63)-Mn(8)-N(19)	100.0(2)
N(12)-Mn(3)-Cl(1)	120.62(14)	N(41)-Mn(8)-N(19)	111.1(2)
N(52)-Mn(4)-N(17)	128.6(2)	N(63)-Mn(8)-N(21)	153.1(2)
N(52)-Mn(4)-N(18)	143.7(2)	N(41)-Mn(8)-N(21)	102.1(2)
N(17)-Mn(4)-N(18)	71.6(2)	N(19)-Mn(8)-N(21)	73.6(2)
N(52)-Mn(4)-N(15)	78.5(2)	N(63)-Mn(8)-N(43)	99.2(2)
N(17)-Mn(4)-N(15)	69.5(2)	N(41)-Mn(8)-N(43)	72.9(2)
N(18)-Mn(4)-N(15)	136.27(19)	N(19)-Mn(8)-N(43)	158.6(2)
N(52)-Mn(4)-N(54)	70.3(2)	N(21)-Mn(8)-N(43)	85.0(2)
N(17)-Mn(4)-N(54)	93.8(2)	N(63)-Mn(8)-N(65)	72.4(2)
N(18)-Mn(4)-N(54)	79.3(2)	N(41)-Mn(8)-N(65)	153.4(2)
N(15)-Mn(4)-N(54)	122.1(2)	N(19)-Mn(8)-N(65)	95.4(2)
N(52)-Mn(4)-Cl(2)	89.05(15)	N(21)-Mn(8)-N(65)	82.0(2)
N(17)-Mn(4)-Cl(2)	138.15(16)	N(43)-Mn(8)-N(65)	81.4(2)
N(18)-Mn(4)-Cl(2)	88.56(14)		

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Complex 3

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Mn(1)-O(1)	2.086(5)	Mn(2)-O(4)#1	2.082(5)
Mn(1)-O(7)	2.169(4)	Mn(2)-O(2)	2.083(5)
Mn(1)-N(2)	2.263(5)	Mn(2)-N(6)	2.197(6)
Mn(1)-N(5)	2.275(6)	Mn(2)-O(5)	2.219(5)
Mn(1)-N(1)	2.278(5)	Mn(2)-O(6)	2.251(5)
Mn(1)-N(9)#1	2.317(5)	Mn(2)-N(10)	2.414(6)
O(1)-Mn(1)-O(7)	89.86(19)	O(4)#1-Mn(2)-O(2)	102.7(2)
O(1)-Mn(1)-N(2)	116.6(2)	O(4)#1-Mn(2)-N(6)	159.1(2)
O(7)-Mn(1)-N(2)	88.32(18)	O(2)-Mn(2)-N(6)	97.5(2)
O(1)-Mn(1)-N(5)	101.7(2)	O(4)#1-Mn(2)-O(5)	88.2(2)
O(7)-Mn(1)-N(5)	95.39(19)	O(2)-Mn(2)-O(5)	86.1(2)
N(2)-Mn(1)-N(5)	141.61(19)	N(6)-Mn(2)-O(5)	87.7(2)
O(1)-Mn(1)-N(1)	171.6(2)	O(4)#1-Mn(2)-O(6)	96.6(2)

O(7)-Mn(1)-N(1)	92.14(17)	O(2)-Mn(2)-O(6)	88.50(18)
N(2)-Mn(1)-N(1)	71.70(19)	N(6)-Mn(2)-O(6)	89.4(2)
N(5)-Mn(1)-N(1)	69.98(19)	O(5)-Mn(2)-O(6)	173.5(2)
O(1)-Mn(1)-N(9)#1	86.6(2)	O(4)#1-Mn(2)-N(10)	89.2(2)
O(7)-Mn(1)-N(9)#1	171.67(19)	O(2)-Mn(2)-N(10)	167.9(2)
N(2)-Mn(1)-N(9)#1	86.6(2)	N(6)-Mn(2)-N(10)	70.9(2)
N(5)-Mn(1)-N(9)#1	92.7(2)	O(5)-Mn(2)-N(10)	96.6(2)
N(1)-Mn(1)-N(9)#1	92.48(18)	O(6)-Mn(2)-N(10)	87.9(2)

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Complex 4

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Mn(1)-O(2)	2.080(4)	Mn(2)-O(1)	2.096(4)
Mn(1)-O(7)	2.212(4)	Mn(2)-O(3)#1	2.112(4)
Mn(1)-N(7)	2.256(4)	Mn(2)-N(3)	2.204(5)
Mn(1)-N(4)	2.260(4)	Mn(2)-O(5)	2.211(5)
Mn(1)-N(6)	2.272(4)	Mn(2)-O(6)	2.262(4)
Mn(1)-N(10)#1	2.325(4)	Mn(2)-N(2)	2.379(5)
O(2)-Mn(1)-O(7)	89.69(17)	O(1)-Mn(2)-O(3)#1	106.21(18)
O(2)-Mn(1)-N(7)	113.30(17)	O(1)-Mn(2)-N(3)	93.79(17)
O(7)-Mn(1)-N(7)	89.07(15)	O(3)#1-Mn(2)-N(3)	159.29(18)
O(2)-Mn(1)-N(4)	104.20(17)	O(1)-Mn(2)-O(5)	87.2(2)
O(7)-Mn(1)-N(4)	93.88(16)	O(3)#1-Mn(2)-O(5)	86.78(18)
N(7)-Mn(1)-N(4)	142.39(15)	N(3)-Mn(2)-O(5)	88.92(19)
O(2)-Mn(1)-N(6)	174.21(17)	O(1)-Mn(2)-O(6)	87.89(16)
O(7)-Mn(1)-N(6)	91.84(15)	O(3)#1-Mn(2)-O(6)	97.65(16)
N(7)-Mn(1)-N(6)	72.32(15)	N(3)-Mn(2)-O(6)	88.24(16)
N(4)-Mn(1)-N(6)	70.12(15)	O(5)-Mn(2)-O(6)	174.15(18)
O(2)-Mn(1)-N(10)#1	86.03(17)	O(1)-Mn(2)-N(2)	163.96(17)
O(7)-Mn(1)-N(10)#1	172.44(16)	O(3)#1-Mn(2)-N(2)	89.48(17)
N(7)-Mn(1)-N(10)#1	86.91(15)	N(3)-Mn(2)-N(2)	70.98(16)
N(4)-Mn(1)-N(10)#1	93.20(16)	O(5)-Mn(2)-N(2)	97.2(2)
N(6)-Mn(1)-N(10)#1	93.03(15)	O(6)-Mn(2)-N(2)	86.66(17)

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Complex 5

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Mn(1)-O(9)	2.135(3)	Mn(3)-N(7)	2.250(4)
Mn(1)-O(9)#1	2.135(3)	Mn(3)-N(6)	2.262(4)
Mn(1)-O(4)#2	2.138(4)	Mn(3)-O(13)	2.270(4)
Mn(1)-O(4)#3	2.139(4)	Mn(4)-O(12)	2.102(4)

Mn(1)-O(2)	2.180(3)	Mn(4)-O(7)#2	2.184(4)
Mn(1)-O(2)#1	2.180(3)	Mn(4)-N(8)	2.188(4)
Mn(2)-O(10)	2.087(4)	Mn(4)-O(6)	2.215(3)
Mn(2)-O(3)#2	2.175(3)	Mn(4)-N(10)	2.354(4)
Mn(2)-N(4)	2.178(4)	Mn(4)-O(5)	2.489(3)
Mn(2)-O(2)	2.215(3)	Mn(5)-O(8)#2	2.125(4)
Mn(2)-N(1)	2.338(4)	Mn(5)-O(8)#4	2.125(4)
Mn(2)-O(1)	2.525(3)	Mn(5)-O(11)	2.133(3)
Mn(3)-O(15)	2.135(4)	Mn(5)-O(11)#5	2.133(3)
Mn(3)-O(14)	2.134(4)	Mn(5)-O(6)#5	2.187(3)
Mn(3)-N(5)	2.249(4)	Mn(5)-O(6)	2.188(3)
O(9)-Mn(1)-O(9)#1	179.999(2)	N(5)-Mn(3)-N(6)	71.41(14)
O(9)-Mn(1)-O(4)#2	94.2(2)	N(7)-Mn(3)-N(6)	70.96(14)
O(9)#1-Mn(1)-O(4)#2	85.8(2)	O(15)-Mn(3)-O(13)	167.1(2)
O(9)-Mn(1)-O(4)#3	85.8(2)	O(14)-Mn(3)-O(13)	79.42(17)
O(9)#1-Mn(1)-O(4)#3	94.2(2)	N(5)-Mn(3)-O(13)	83.61(16)
O(4)#2-Mn(1)-O(4)#3	179.998(1)	N(7)-Mn(3)-O(13)	101.29(18)
O(9)-Mn(1)-O(2)	89.69(13)	N(6)-Mn(3)-O(13)	83.36(17)
O(9)#1-Mn(1)-O(2)	90.31(13)	O(12)-Mn(4)-O(7)#2	92.77(16)
O(4)#2-Mn(1)-O(2)	83.03(14)	O(12)-Mn(4)-N(8)	105.04(15)
O(4)#3-Mn(1)-O(2)	96.97(14)	O(7)#2-Mn(4)-N(8)	99.13(17)
O(9)-Mn(1)-O(2)#1	90.31(13)	O(12)-Mn(4)-O(6)	98.32(14)
O(9)#1-Mn(1)-O(2)#1	89.69(13)	O(7)#2-Mn(4)-O(6)	113.64(17)
O(4)#2-Mn(1)-O(2)#1	96.97(14)	N(8)-Mn(4)-O(6)	138.50(13)
O(4)#3-Mn(1)-O(2)#1	83.03(14)	O(12)-Mn(4)-N(10)	177.04(15)
O(2)-Mn(1)-O(2)#1	180.0	O(7)#2-Mn(4)-N(10)	85.48(15)
O(10)-Mn(2)-O(3)#2	93.01(15)	N(8)-Mn(4)-N(10)	72.94(14)
O(10)-Mn(2)-N(4)	106.64(14)	O(6)-Mn(4)-N(10)	84.57(13)
O(3)#2-Mn(2)-N(4)	100.00(16)	O(12)-Mn(4)-O(5)	90.33(15)
O(10)-Mn(2)-O(2)	97.95(14)	O(7)#2-Mn(4)-O(5)	168.47(17)
O(3)#2-Mn(2)-O(2)	114.84(15)	N(8)-Mn(4)-O(5)	90.77(13)
N(4)-Mn(2)-O(2)	135.93(12)	O(6)-Mn(4)-O(5)	54.87(11)
O(10)-Mn(2)-N(1)	177.92(15)	N(10)-Mn(4)-O(5)	91.84(13)
O(3)#2-Mn(2)-N(1)	85.16(14)	O(8)#2-Mn(5)-O(8)#4	180.0
N(4)-Mn(2)-N(1)	72.77(13)	O(8)#2-Mn(5)-O(11)	94.0(2)

O(2)-Mn(2)-N(1)	83.73(12)	O(8)#4-Mn(5)-O(11)	86.0(2)
O(10)-Mn(2)-O(1)	89.34(14)	O(8)#2-Mn(5)-O(11)#5	86.0(2)
O(3)#2-Mn(2)-O(1)	169.46(15)	O(8)#4-Mn(5)-O(11)#5	94.0(2)
N(4)-Mn(2)-O(1)	89.15(12)	O(11)-Mn(5)-O(11)#5	180.0
O(2)-Mn(2)-O(1)	54.63(11)	O(8)#2-Mn(5)-O(6)#5	96.94(15)
N(1)-Mn(2)-O(1)	92.64(13)	O(8)#4-Mn(5)-O(6)#5	83.06(15)
O(15)-Mn(3)-O(14)	94.9(2)	O(11)-Mn(5)-O(6)#5	89.34(13)
O(15)-Mn(3)-N(5)	90.32(17)	O(11)#5-Mn(5)-O(6)#5	90.66(13)
O(14)-Mn(3)-N(5)	124.60(18)	O(8)#2-Mn(5)-O(6)	83.06(15)
O(15)-Mn(3)-N(7)	90.60(18)	O(8)#4-Mn(5)-O(6)	96.94(15)
O(14)-Mn(3)-N(7)	94.01(18)	O(11)-Mn(5)-O(6)	90.66(13)
N(5)-Mn(3)-N(7)	141.14(14)	O(11)#5-Mn(5)-O(6)	89.34(13)
O(15)-Mn(3)-N(6)	105.6(2)	O(6)#5-Mn(5)-O(6)	180.00(13)
O(14)-Mn(3)-N(6)	154.45(18)		

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Complex 6

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Mn(1)-O(1)	2.087(3)	Mn(2)-O(2)	2.095(3)
Mn(1)-O(4)#1	2.094(3)	Mn(2)-O(8)	2.225(3)
Mn(1)-N(8)	2.172(3)	Mn(2)-N(7)	2.226(3)
Mn(1)-N(3)#2	2.222(3)	Mn(2)-O(7)	2.237(3)
Mn(1)-N(2)#2	2.322(3)	Mn(2)-N(6)	2.253(3)
Mn(1)-N(10)	2.464(4)	Mn(2)-N(5)	2.264(3)
O(1)-Mn(1)-O(4)#1	92.62(12)	O(2)-Mn(2)-O(8)	86.94(11)
O(1)-Mn(1)-N(8)	101.38(12)	O(2)-Mn(2)-N(7)	110.50(12)
O(4)#1-Mn(1)-N(8)	97.92(13)	O(8)-Mn(2)-N(7)	89.68(12)
O(1)-Mn(1)-N(3)#2	96.24(12)	O(2)-Mn(2)-O(7)	96.23(12)
O(4)#1-Mn(1)-N(3)#2	159.52(12)	O(8)-Mn(2)-O(7)	172.40(11)
N(8)-Mn(1)-N(3)#2	98.37(13)	N(7)-Mn(2)-O(7)	82.74(13)
O(1)-Mn(1)-N(2)#2	97.01(12)	O(2)-Mn(2)-N(6)	175.13(12)
O(4)#1-Mn(1)-N(2)#2	87.73(12)	O(8)-Mn(2)-N(6)	88.68(11)
N(8)-Mn(1)-N(2)#2	160.45(12)	N(7)-Mn(2)-N(6)	71.59(11)
N(3)#2-Mn(1)-N(2)#2	72.91(11)	O(7)-Mn(2)-N(6)	88.38(12)
O(1)-Mn(1)-N(10)	170.74(12)	O(2)-Mn(2)-N(5)	105.44(12)
O(4)#1-Mn(1)-N(10)	85.08(13)	O(8)-Mn(2)-N(5)	93.79(11)
N(8)-Mn(1)-N(10)	70.15(12)	N(7)-Mn(2)-N(5)	144.02(12)
N(3)#2-Mn(1)-N(10)	88.86(12)	O(7)-Mn(2)-N(5)	92.02(12)

N(2)#2-Mn(1)-N(10)	91.87(11)	N(6)-Mn(2)-N(5)	72.71(12)
Complex 7			
Mn(1)-O(2)	2.090(4)	Mn(2)-O(1)	2.134(3)
Mn(1)-N(3)	2.223(3)	Mn(2)-O(6)	2.195(3)
Mn(1)-N(10)#2	2.318(4)	Mn(2)-N(4)	2.296(3)
Mn(1)-O(4)#1	2.103(3)	Mn(2)-O(5)	2.172(3)
Mn(1)-N(8)#2	2.258(3)	Mn(2)-N(6)	2.278(3)
Mn(1)-N(1)	2.380(4)	Mn(2)-N(7)	2.447(3)
O(2)-Mn(1)-O(4)#1	108.61(17)	O(1)-Mn(2)-O(5)	84.19(13)
O(4)#1-Mn(1)-N(3)	98.36(12)	O(1)-Mn(2)-O(6)	83.36(13)
O(4)#1-Mn(1)-N(8)#2	91.69(12)	O(1)-Mn(2)-N(6)	169.24(12)
O(2)-Mn(1)-N(10)#2	89.51(17)	O(6)-Mn(2)-N(6)	106.29(12)
N(3)-Mn(1)-N(10)#2	91.91(12)	O(5)-Mn(2)-N(4)	99.78(12)
O(2)-Mn(1)-N(1)	153.18(13)	N(6)-Mn(2)-N(4)	71.48(11)
N(3)-Mn(1)-N(1)	72.08(12)	O(5)-Mn(2)-N(7)	87.77(12)
N(10)#2-Mn(1)-N(1)	80.75(13)	N(6)-Mn(2)-N(7)	69.28(11)
O(2)-Mn(1)-N(3)	83.43(13)	O(5)-Mn(2)-O(6)	157.53(12)
O(2)-Mn(1)-N(8)#2	112.14(14)	O(5)-Mn(2)-N(6)	88.11(12)
N(3)-Mn(1)-N(8)#2	157.76(12)	O(1)-Mn(2)-N(4)	102.42(12)
O(4)#1-Mn(1)-N(10)#2	160.00(13)	O(6)-Mn(2)-N(4)	101.13(13)
N(8)#2-Mn(1)-N(10)#2	73.16(12)	O(1)-Mn(2)-N(7)	117.75(12)
O(4)#1-Mn(1)-N(1)	86.12(13)	O(6)-Mn(2)-N(7)	81.60(12)
N(8)#2-Mn(1)-N(1)	88.97(12)	N(4)-Mn(2)-N(7)	139.71(11)

Symmetry transformations used to generate equivalent atoms for complex **1**: #1  $-x+1, y+1/2, -z+1$ . For complex **3**: #1  $x, -y+3/2, z-1/2$ . For complex **4**: #1  $x, -y+3/2, z+1/2$ . For complex **5**: #1  $-x+1, -y+1, -z+1$ ; #2  $x+1, y, z$ ; #3  $-x, -y+1, -z+1$ ; #4  $-x, -y+1, -z$ ; #5  $-x+1, -y+1, -z$ . For complex **6**: #1  $x, y+1, z$ ; #2  $x, -y+3/2, z-1/2$ . For complex **7**: #1  $y+1/2, -x+1, z-1/2$ ; #2  $-y+1, x-1/2, z-1/2$ .



## 6. Table for the selected hydrogen bonds.

**Table S3.** Selected hydrogen bonds for complex **1**, **3**, **4** and **6**.

Complex 1				
D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (°)
O(2)-H(3W)...Cl(2)#2	0.85	2.47	3.062(3)	127.1
O(3)-H(6W)...Cl(2)#2	0.85	2.94	3.789(5)	179.8
Complex 3				
D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (°)
O(5)-H(1W)...O(3)#3	0.85	1.84	2.598(8)	148.0
O(5)-H(2W)...O(5)#4	0.85	2.32	2.757(11)	112.4
O(7)-H(6W)...O(3)#3	0.85	2.00	2.844(7)	176.0
Complex 4				
D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (°)
O(5)-H(1W)...O(5)#2	0.85	2.36	2.824(10)	114.9
O(5)-H(2W)...O(4)#3	0.85	1.79	2.583(7)	153.9
O(7)-H(6W)...O(4)#3	0.85	2.20	2.990(6)	154.5
Complex 6				
D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	<(DHA) (°)
O(5)-H(5)...N(1)#3	0.82	2.01	2.811(6)	163.9

Symmetry transformations used to generate equivalent atoms for complex **1**: #2 -x+1, y-1/2, -z. For complex **3**: #3 -x, y+1/2, -z+1/2;

#4 -x, -y+2, -z. For complex **4**: #2 -x+1, -y+2, -z+1; #3 -x+1, y+1/2, -z+1/2. For complex **6**: #3 -x+1, -y+1, -z+1.