Electronic Supplementary Material (ESI) for CrystEngComm.

A functional nitroxide ligand build up two 2p-3d complexes with different spin ground states and a 2p-3d-4f chain of rings

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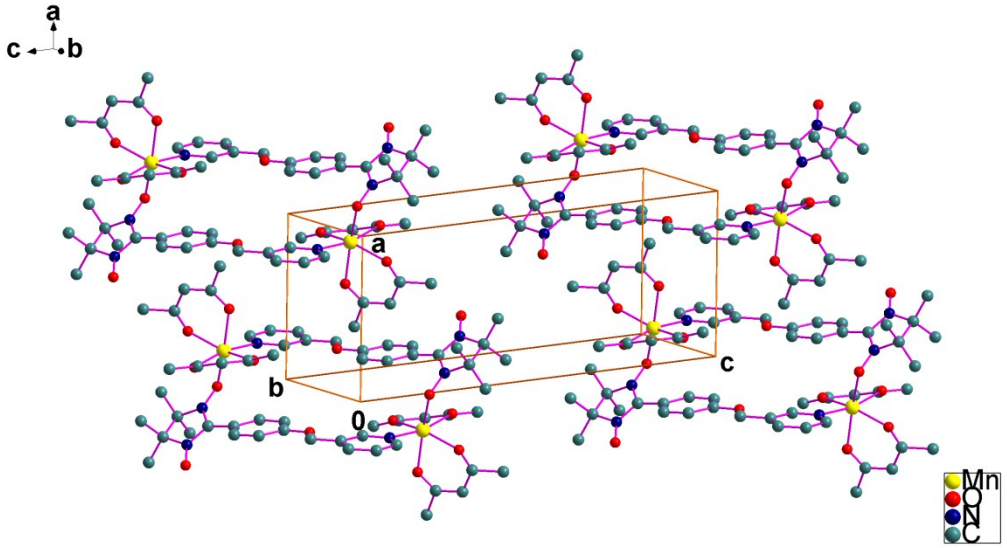


Figure S1. Packing arrangement of complex **1** down the c-axis.

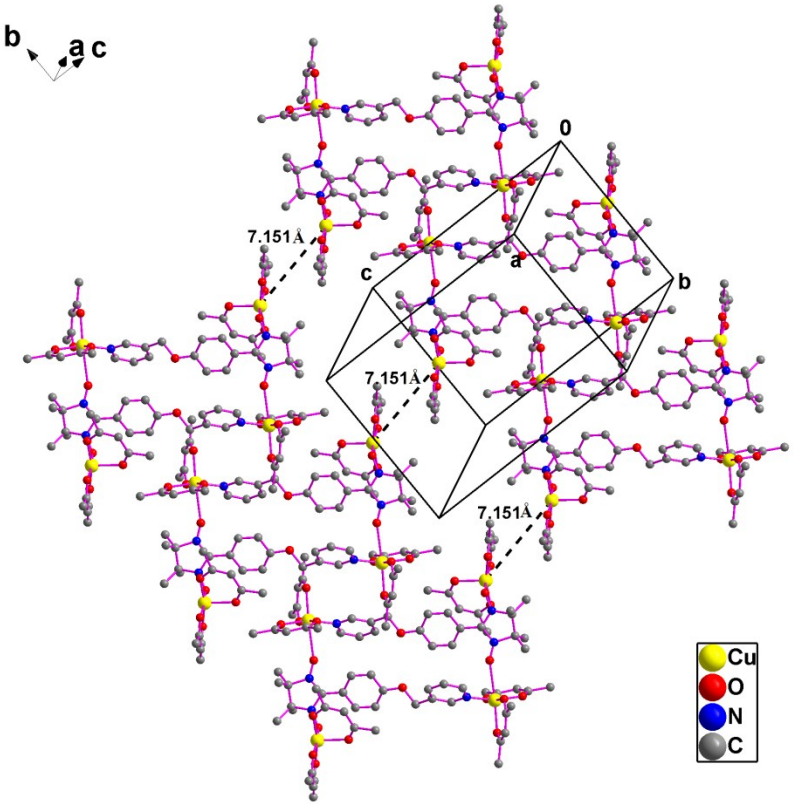


Figure S2. Packing arrangement of complex **2**.

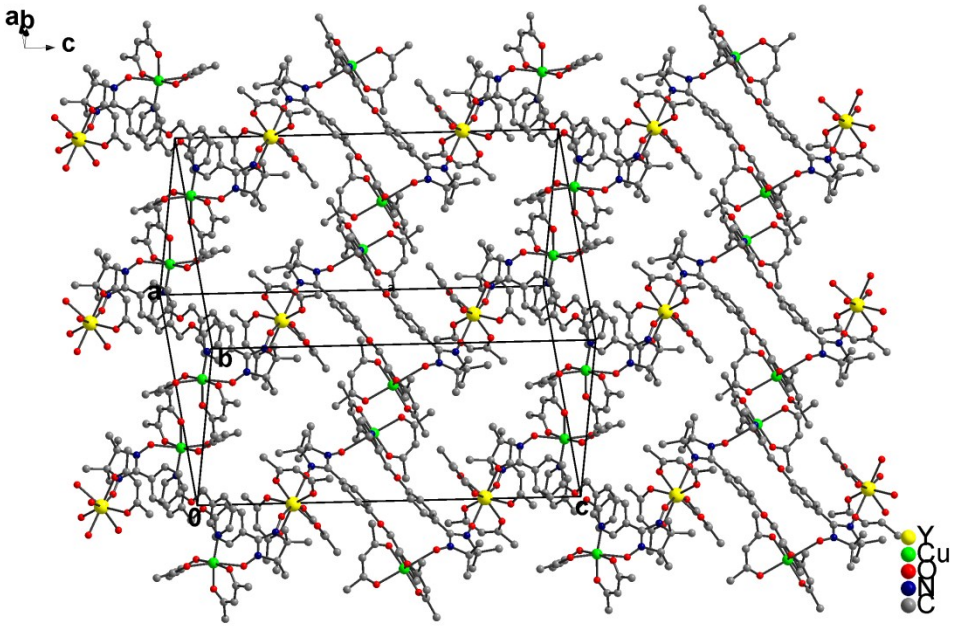


Figure S3. Packing of the chains in crystal for complex **3**.

Table S1 Selected bond lengths (Å) and angles (°) for complexes **1-3**

Complex **1**		Complex **2**		Complex **3**	
Mn(1) –O(1)	2.182(4)	Cu(1) –O(1)	1.970(3)	Y(1) –O(1)	2.314(5)
Mn(1) –O(3)	2.133(5)	Cu(1) –O(3)	2.231(3)	Y(1) –O(2)	2.344(5)
Mn(1) –O(5)	2.152(5)	Cu(1) –O(6)	2.748(3)	Y(1) –O(3)	2.345(5)
Mn(1) –O(2)	2.165(4)	Cu(2) –O(7)	1.943(3)	Y(1) –O(4)	2.317(5)
Mn(1) –O(4)	2.200(5)	Cu(2) –O(9)	2.208(3)	Cu(1) –O(5)	2.662(6)
Mn(1)-N(3)	2.209(5)	Cu(2) –O(11)	1.942(3)	Cu(1) –O(8)	2.270(6)
O(2)-Mn(1)-O(5)	91.27(17)	Cu(1) –O(2)	1.944(3)	Cu(1) –O(10)	1.964(5)
O(4)-Mn(1)-O(5)	166.39(16)	Cu(1) –O(4)	1.949(3)	Cu(1) –O(7)	1.954(5)
O(1)-Mn(1)-O(5)	111.57(18)	Cu(1)–N(1)	2.010(3)	Cu(1) –O(9)	1.951(5)
O(4)-Mn(1)-N(3)	92.13(18)	Cu(2)–O(8)	1.937(3)	Cu(1) –N(3)	2.004(6)
O(3)-Mn(1)-N(3)	103.72(18)	Cu(2) –O(10)	1.980(3)	O(4)-Y(1)-O(1)	107.06(18)
O(3)-Mn(1)-O(4)	81.27(19)	O(6)-Cu(1)-N(1)	75.688(12)	O(4)-Y(1)-O(3)	71.16(18)
O(2)-Mn(1)-O(4)	97.82(17)	N(1)-Cu(1)-O(4)	92.19(13)	O(4)-Y(1)-O(2)	73.80(18)
O(2)-Mn(1)-O(1)	81.63(16)	N(1)-Cu(1)-O(3)	99.29(13)	O(4)-Y(1)-O(4)#1	135.4(3)
O(4)-Mn(1)-O(1)	79.92(17)	O(2)-Cu(1)-N(1)	89.23(13)	O(5)-Cu(1)-O(7)	93.1(2)
O(1)-Mn(1)-O(3)	154.77(18)	O(8)-Cu(2)-O(7)	92.94(13)	O(5)-Cu(1)-O(9)	74.1(2)
O(1)-Mn(1)-N(3)	93.66(18)	O(7)-Cu(2)-O(9)	101.99(12)	O(5)-Cu(1)-N(3)	90.2(2)
O(2)-Mn(1)-N(3)	168.04(19)	O(11)-Cu(2)-O(7)	82.73(13)	N(3)-Cu(1)-O(8)	101.0(2)
O(5)-Mn(1)-N(3)	80.20(18)	O(7)-Cu(2)-O(10)	171.22(12)	N(3)-Cu(1)-O(10)	92.9(2)
N(1)-O(5)-Mn(1)	122.5(4)	N(2)-O(6)-Cu(1)	159.2(2)	N(1)-O(4)-Y(1)	141.8(4)
		N(3)-O(7)-Cu(2)	119.1(2)	N(2)-O(5)-Cu(1)	133.5(5)

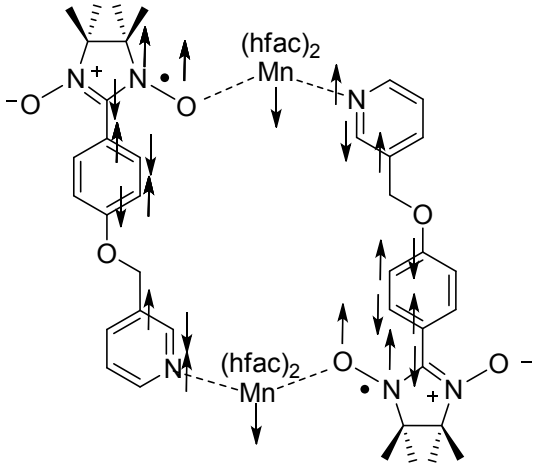
Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2

Table S2. Results of continuous shape measures analysis for the metal coordination spheres

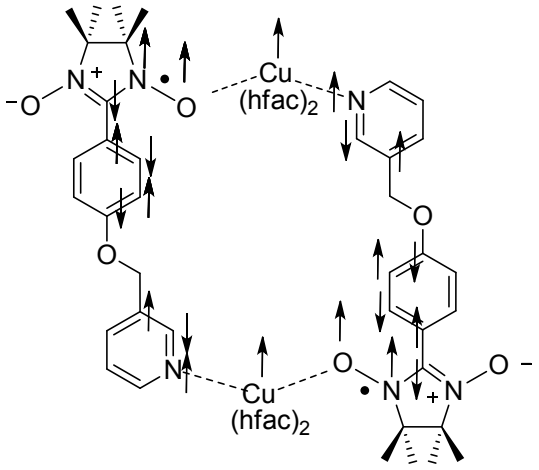
Complex	Metal	OC-6	TPR-6	PPY-6
1	Mn	**2.504**	7.834	20.959

Complex	Metal	OC-6	TPR-6	PPY-6	SPY-5	vOC-5	TBPY-5
2	Cu1	**1.874**	15.691	26.994			
	Cu2				**1.040**	1.344	5.352

Complex	Metal	TDD-8	SAPR-8	BTPR-8	OC-6	TPR-6	PPY-6
3	Y	**0.637**	1.004	2.118			
	Cu				**2.087**	14.215	24.768



Scheme S1. Spin parity analysis for the spin-spin interaction of complex **1**.



Scheme S2. Spin parity analysis for the spin-spin interaction of complex **2**.

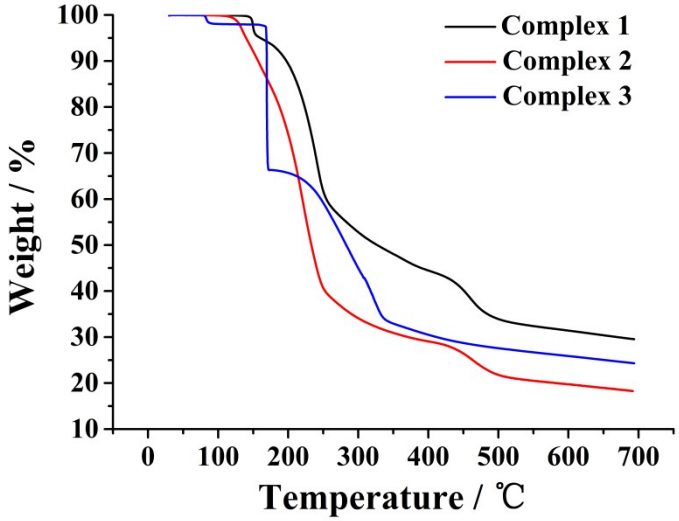


Figure S4 Thermal analysis curve of the complexes **1-3**