Electronic Supplementary Material (ESI) for Dalton Transactions

Synthesis, structural characterization and anion-sensing studies of metal(II) complexes based on 3, 3', 4, 4'-oxydiphthalate and N-donor ligands

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Table S1 Selected bond lengths (Å) and angles (°) for complexes **1-5**

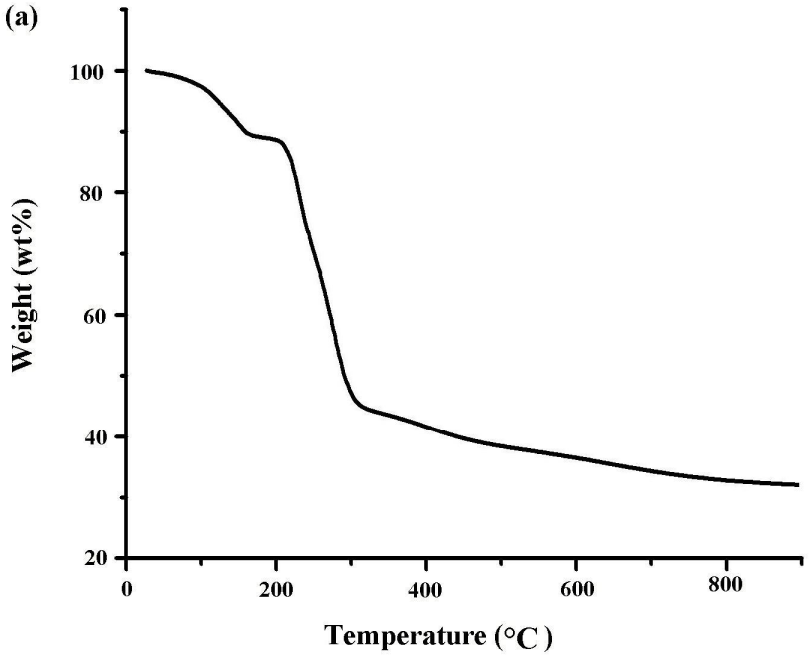
Complex 1			
Cu(1)-N(3)	2.026(3)	Cu(1)-N(2)#1	2.024(3)
Cu(1)-N(4)	2.013(3)	Cu(1)-O(1)	1.973(2)
Cu(1)-O(10)	2.335(3)	Cu(3)-N(1) #3	1.990(3)
Cu(3)-O(9)	1.938(3)	Cu(2)-O(12)	2.114(3)
Cu(2)-O(13)	2.081(3)	Cu(2)-O(11)	2.146(3)
N(3)-Cu(1)-N(2) #1	86.95(1)	N(4)-Cu(1)-N(3)	92.15(1)
N(4)-Cu(1)-N(2) #1	175.02(1)	O(1)-Cu(1)-O(10)	94.76(1)
O(9)-Cu(3)-N(1)#3	87.66(1)	O(9)-Cu(3)-O(9)#2	180.0(6)
O(13)-Cu(2)-O(12)#4	87.72(1)	O(11)#4-Cu(2)-O(11)	180.00(2)
Complex 2			
Co(1)-N(1)	2.1066(2)	Co(1)-N(1)#5	2.1066(2)

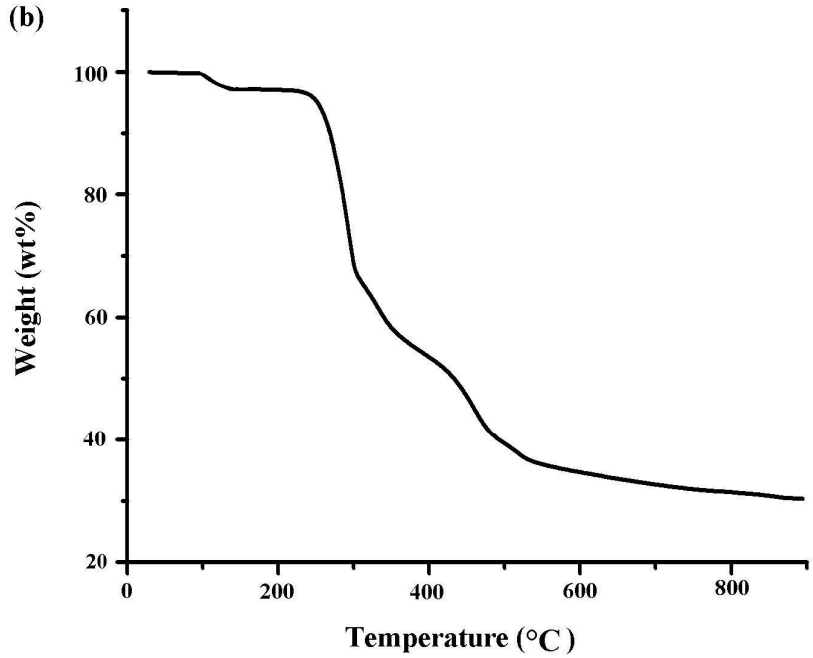
Co(1)-O(6)	2.2435(8)	Co(1)-O(1)	2.0601(1)
O(1)-Co(1)-O(6)	92.28(6)	N(1)-Co(1)-O(6)	92.00(5)
O(1)-Co(1)-N(1)	90.08(6)	C(7)-O(1)-Co(1)	129.28(1)
Complex 3			
Zn(1)-O(7)	1.991(3)	Zn(1)-O(1)	1.946(3)
Zn(1)-O(9)	1.956(3)	Zn(1)-O(6)	1.975(3)
O(6)-Zn(1)-O(7)	95.52(1)	O(9)-Zn(1)-O(7)	129.56(1)
O(1)-Zn(1)-O(6)	114.47(1)	O(1)-Zn(1)-O(7)	101.56(1)
Complex 4			
Mn(1)-N(1)	2.301(4)	Mn(1)-N(2)	2.291(4)
Mn(1)-O(7)	2.179(3)	Mn(1)-O(6)	2.231(3)
Mn(2)-O(9)	2.046(4)	Mn(2)-O(10)#6	2.496(7)
O(7)-Mn(1)-O(6)	79.37(1)	O(1)-Mn(1)-O(6)	167.65(1)
N(2)-Mn(1)-N(1)	72.17(1)	O(7)-Mn(1)-N(1)	83.44(1)
O(9)-Mn(2)-O(11)	125.4(3)	O(3)-Mn(2)-O(10)	140.7(2)
Complex 5			
Cu(1)-O(1)	2.0124(2)	Cu(1)-N(4)	1.9759(2)
Cu(1)-N(3)	2.068(2)	Cu(1)-N(2)	2.149(2)
N(4)-Cu(1)-N(1)	175.77(8)	N(1)-Cu(1)-O(1)	88.86(7)
N(1)-Cu(1)-N(2)	80.76(8)	N(3)-Cu(1)-N(2)	116.82(7)

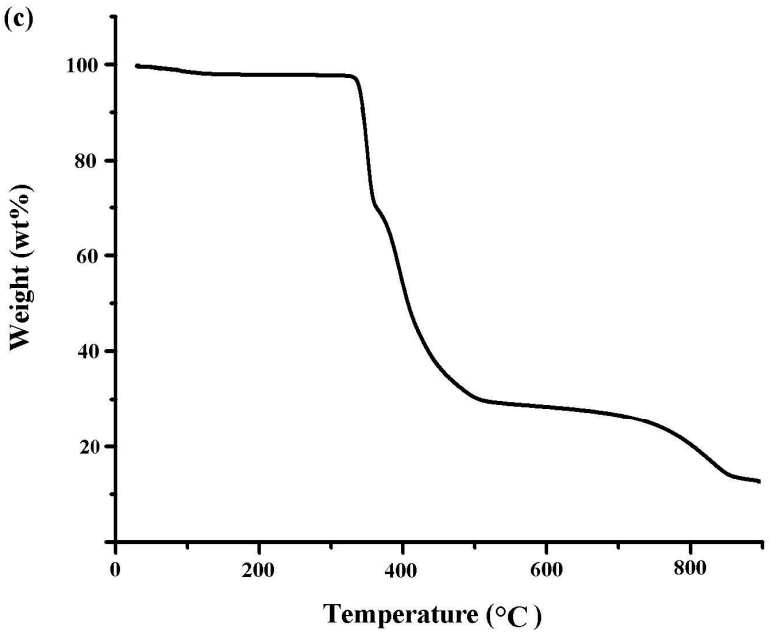
Symmetry transformations used to generate equivalent atoms:

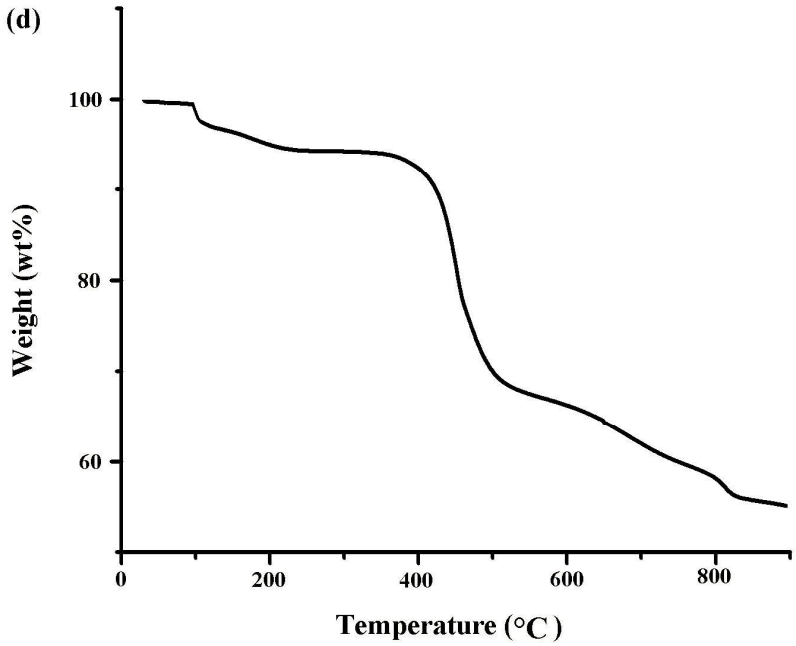
#1 x-1,y,z #2 -x,-y,-z+1 #3 -x,-y+1,-z

#4 -x+1,-y+2,-z+1 #5 -x,-y+1,-z #6 -x,-y+1,-z+1









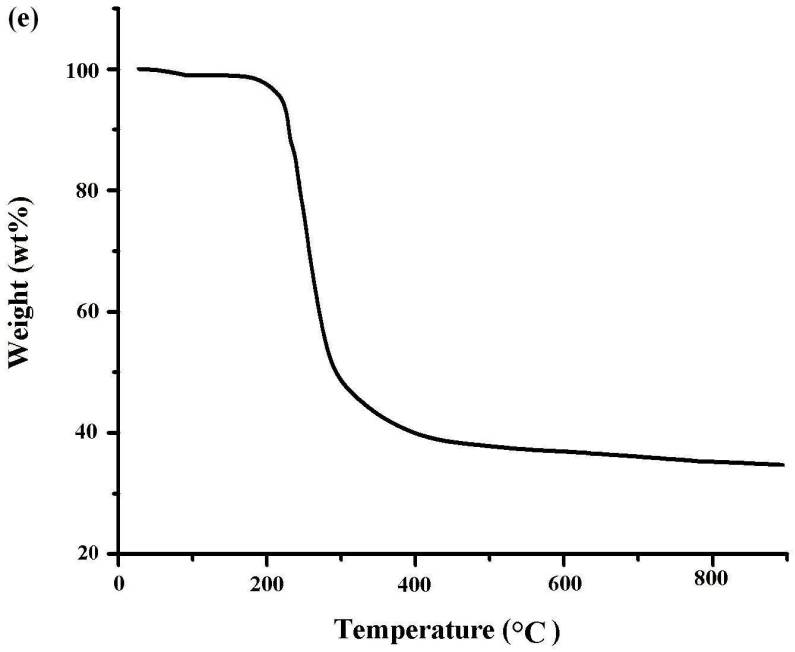


Fig. S1 Thermogravimetric carves of complexes **1**(**a**), **2**(**b**), **3**(**c**), **4**(**d**) and **5**(**e**).

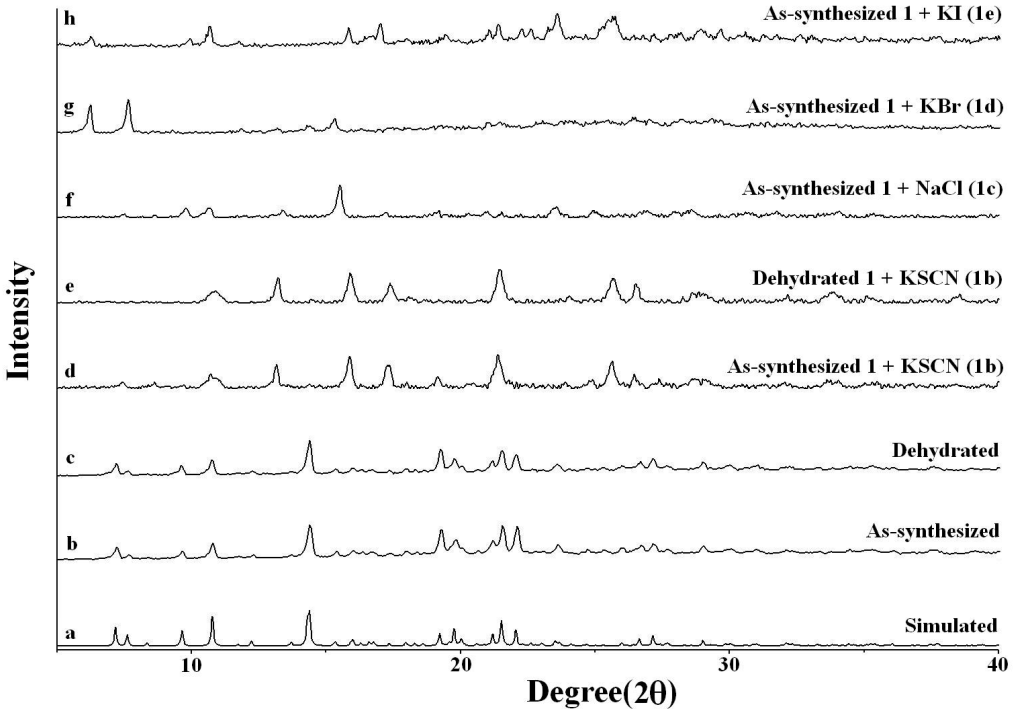


Fig.S2 PXRD patterns of simulated from the X-ray single structure of **1** (**a**), as-synthesized **1** (**b**), dehydrated **1** (**c**), and diffraction patterns obtained after the introduction of different anions: as-synthesized **1** + KSCN (**d**), dehydrated **1** + KSCN (**e**), as-synthesized **1** + NaCl (**f**), as-synthesized **1** + KBr (**g**) and as-synthesized **1** + KI (**h**).

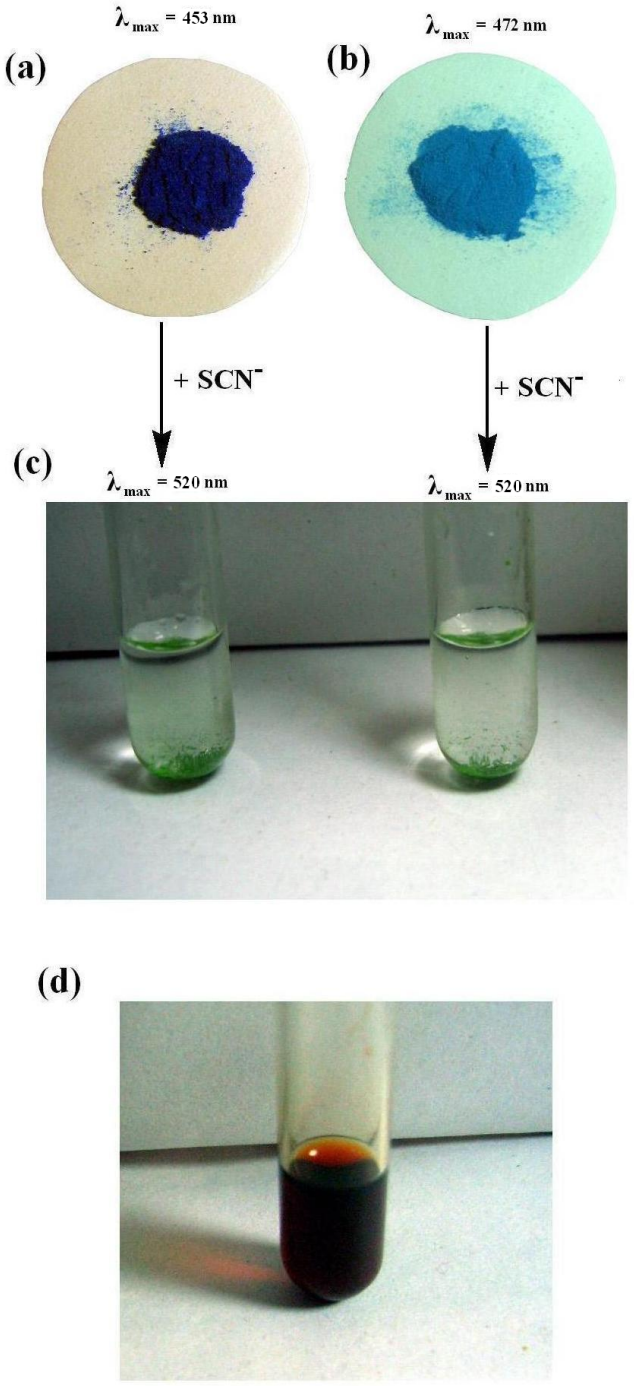


Fig.S3 The as-synthesized (blue) (**a**) and dehydrated (sapphire) complex **1** (**b**), the green solid sample **1b** obtained upon the addition of SCN^- to the as-synthesized and dehydrated

complex **1** (**c**) and the blood-red suspension obtained upon the addition of Fe^{3+} to **1b** (**d**). λ_{max}: the maximal reflection wavelength of the solid sample in the UV-vis spectrum.

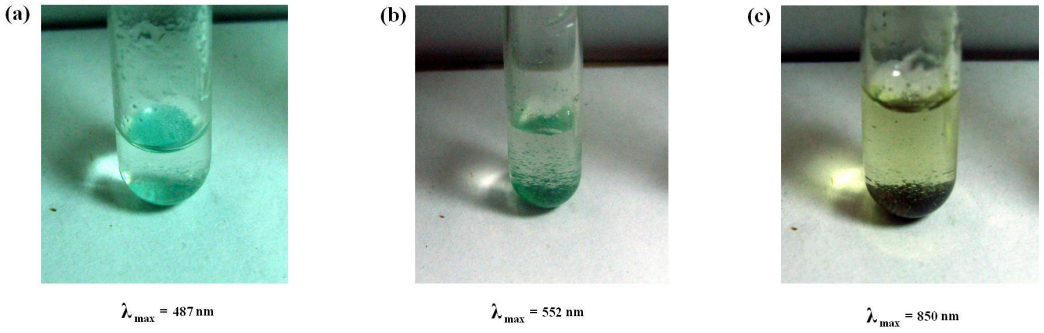


Fig. S4 The sky-blue **1c** (**a**), grass-green **1d** (**b**) and brown solid samples **1e** (**c**) obtained upon the addition of Cl^-, Br^- and I^- to the as-synthesized **1**, respectively. λ_{max}: the maximal reflection wavelength of the solid sample in the UV-vis spectrum.

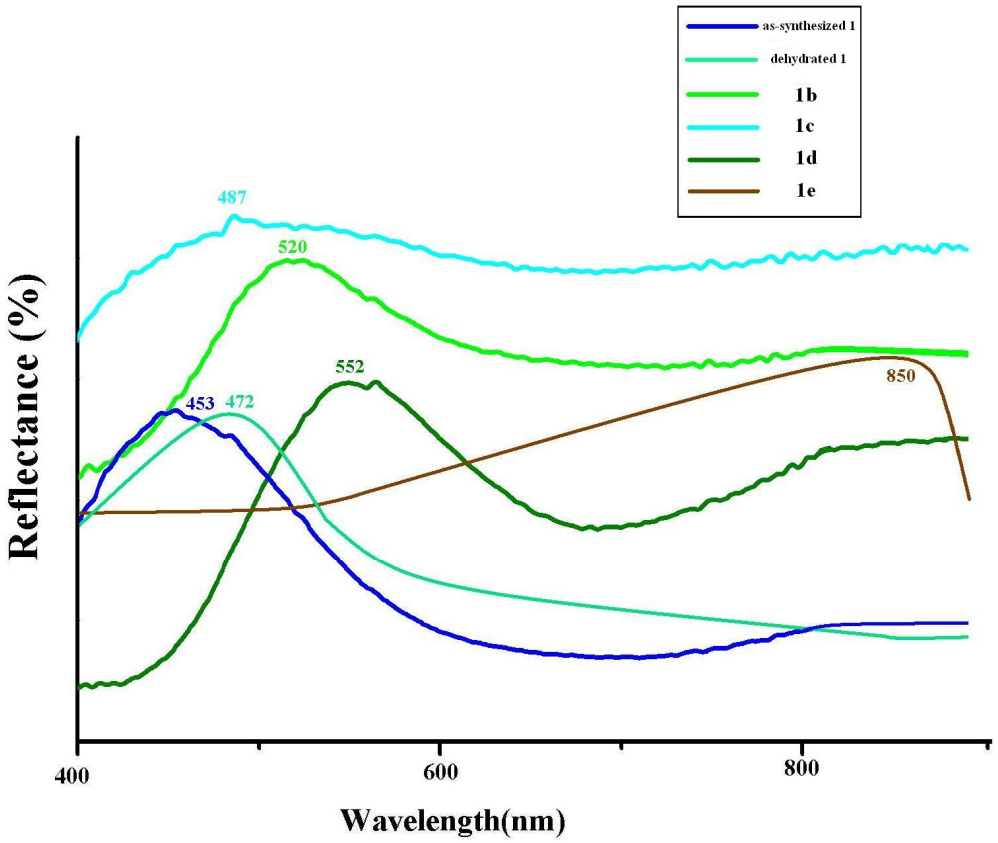
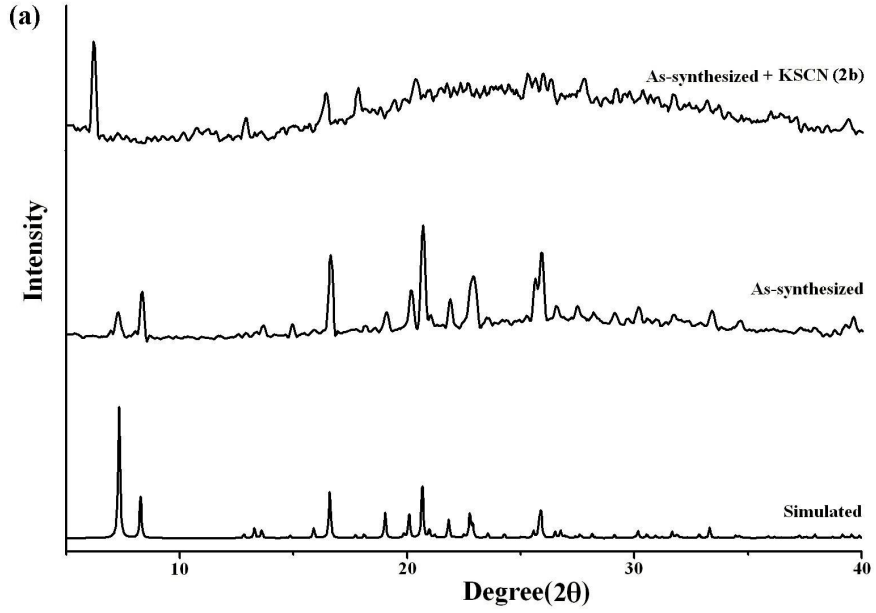
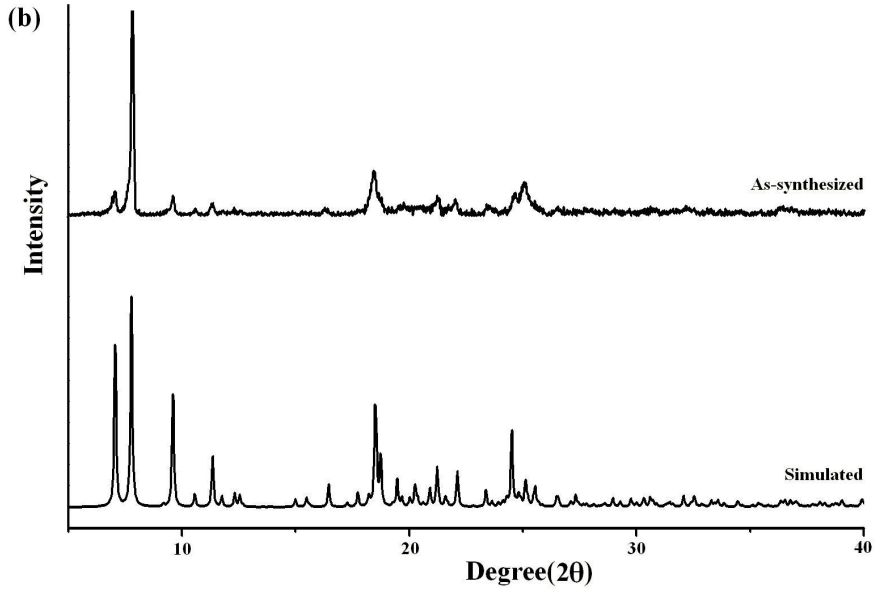


Fig. S5 The UV-vis spectra of as-synthesized **1**, dehydrated **1**, **1b**, **1c**, **1d** and **1e**.





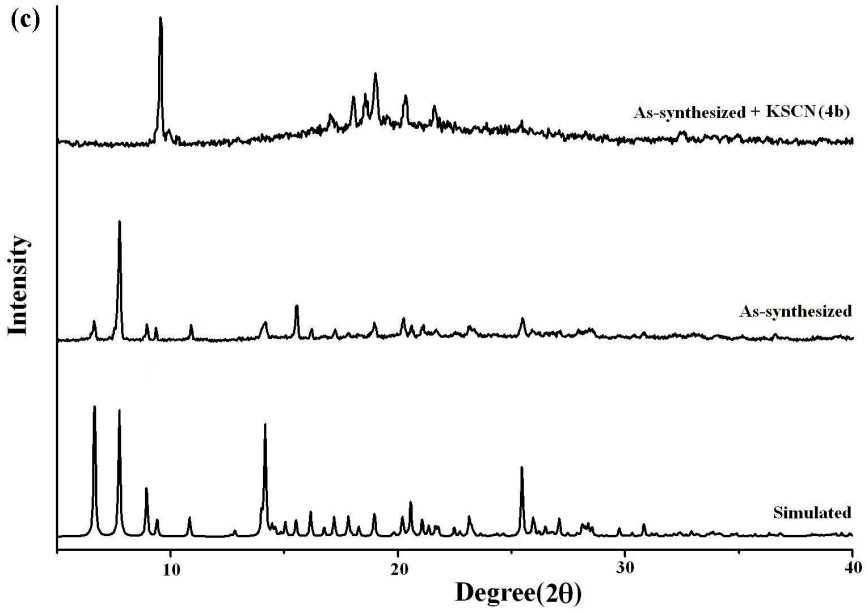


Fig.S6 The PXRD patterns of complexes **2** (**a**), **3** (**b**) and **4** (**c**). PXRD patterns of simulated from the X-ray single structure (**bottom**), as-synthesized (**middle**) and diffraction patterns obtained after the introduction of KSCN (**above**).

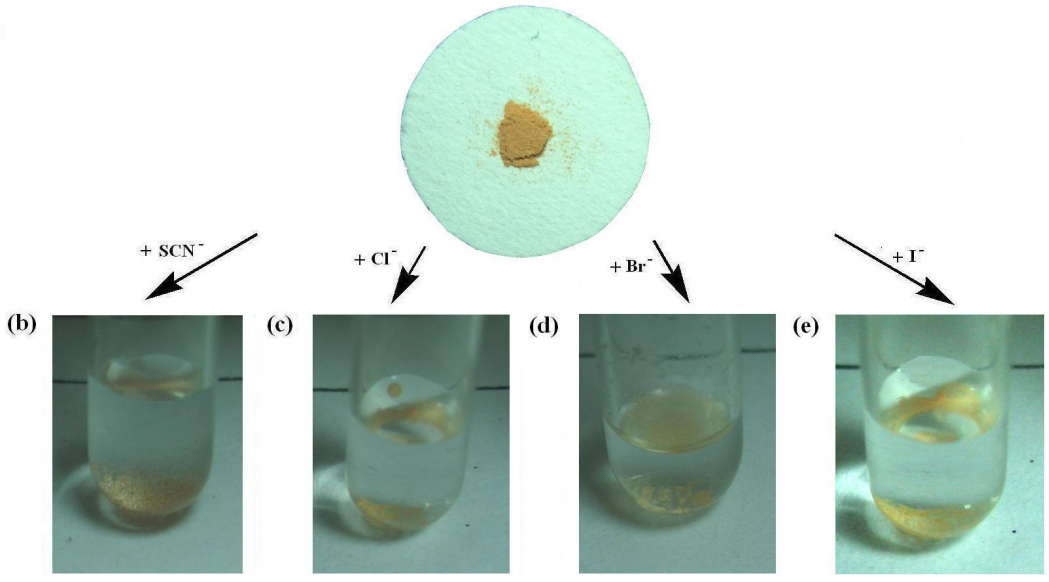


Fig. S7 The as-synthesized complex **2** (**a**) and the solid samples obtained upon the

addition of SCN^-(**b**), Cl^- (**c**), Br^- (**d**) and I^- (**e**) to the as-synthesized **2**, respectively.

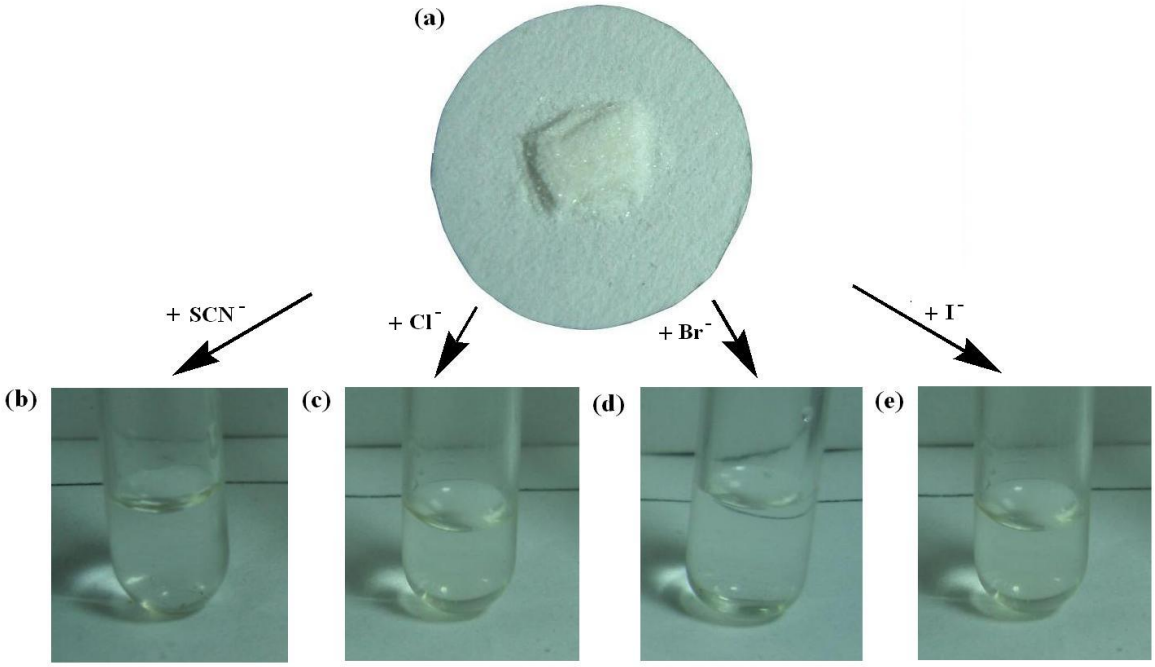


Fig.S8 The as-synthesized complex **3** (**a**) and the colorless solution obtained upon the addition of SCN^-(**b**), Cl^- (**c**), Br^- (**d**) and I^- (**e**) to the as-synthesized **3**, respectively.

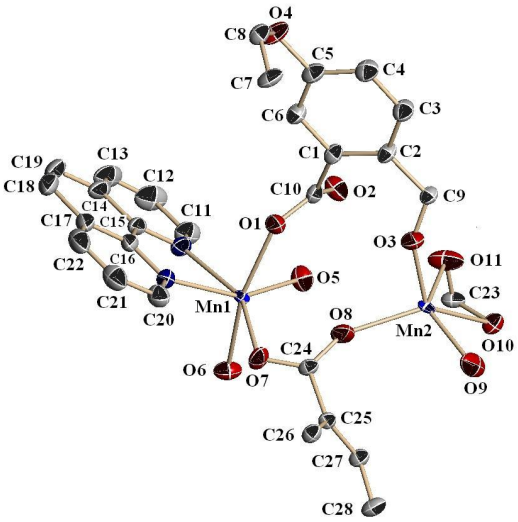


Fig.S9 ORTEP drawing of $Mn_2(ODPA)(phen)(H_2O)_2$ (**4**) with thermal ellipsoids at 50% probability (H and disordered O atoms omitted for clarity)

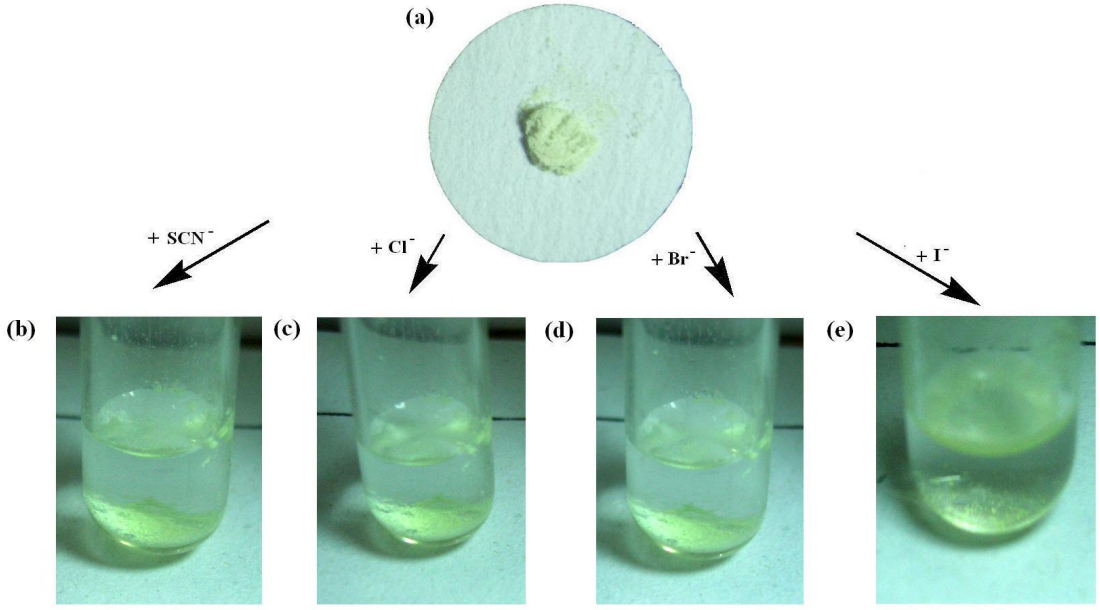


Fig. S10 The as-synthesized complex **4** (**a**) and the solid samples obtained upon the addition of SCN^-(**b**), Cl^- (**c**), Br^- (**d**) and I^- (**e**) to the as-synthesized **4**, respectively.

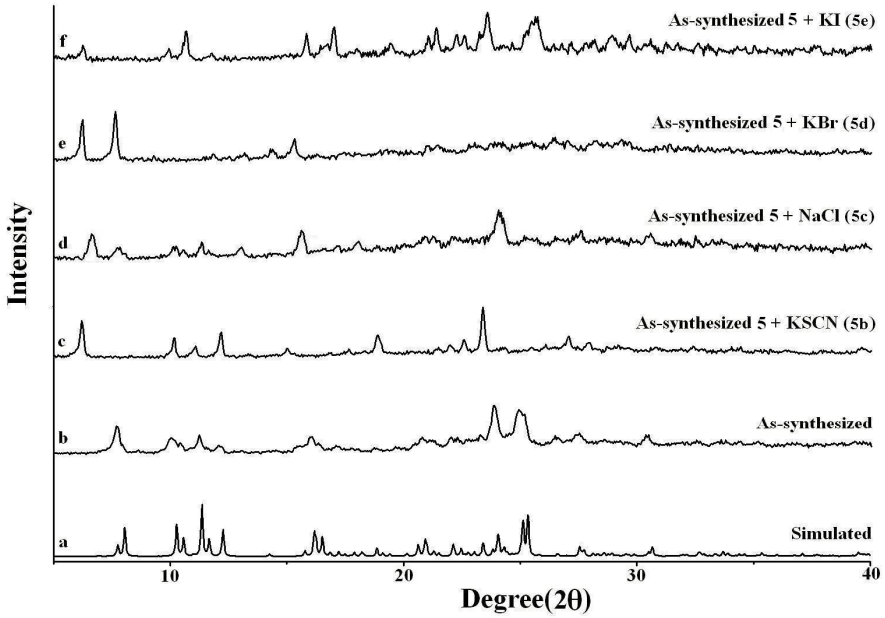


Fig. S11 PXRD patterns of simulated from the X-ray single structure of **5** (**a**), as-synthesized **5** (**b**) and diffraction patterns obtained after the introduction of different anions: as-synthesized **5** + KSCN (**c**), as-synthesized **5** + NaCl (**d**), as-synthesized **5** + KBr (**e**) and as-synthesized **1** + KI (**f**).

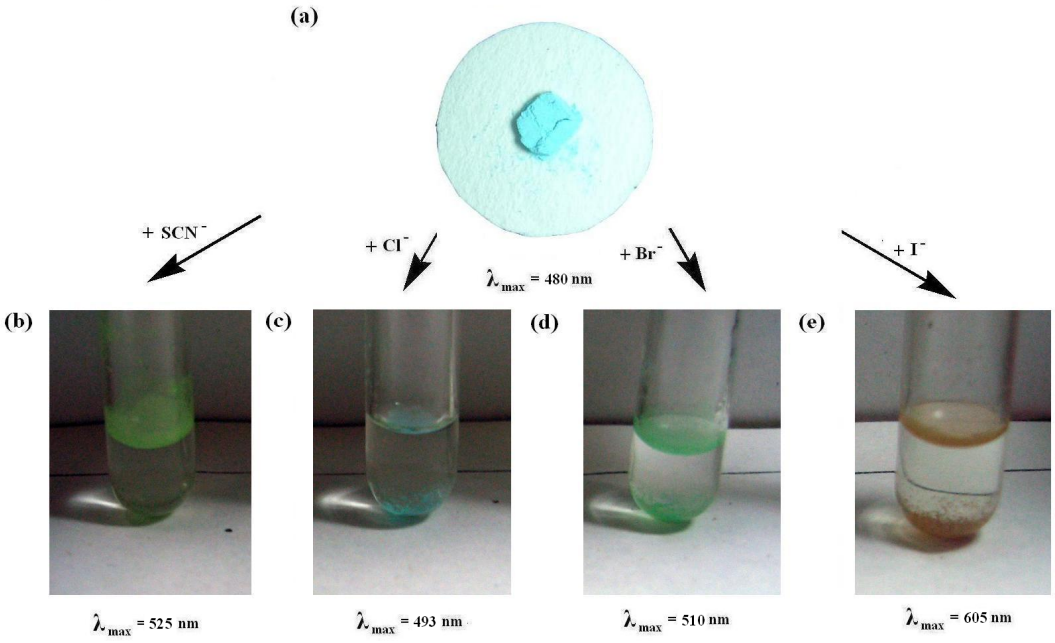


Fig. S12 The as-synthesized complex **5** (**a**) and the solid samples obtained upon the addition of SCN^-(**b**), Cl^- (**c**), Br^- (**d**) and I^- (**e**) to the as-synthesized **5**, respectively. λ_{max}: the maximal reflection wavelength of the solid sample in the UV-vis spectrum.

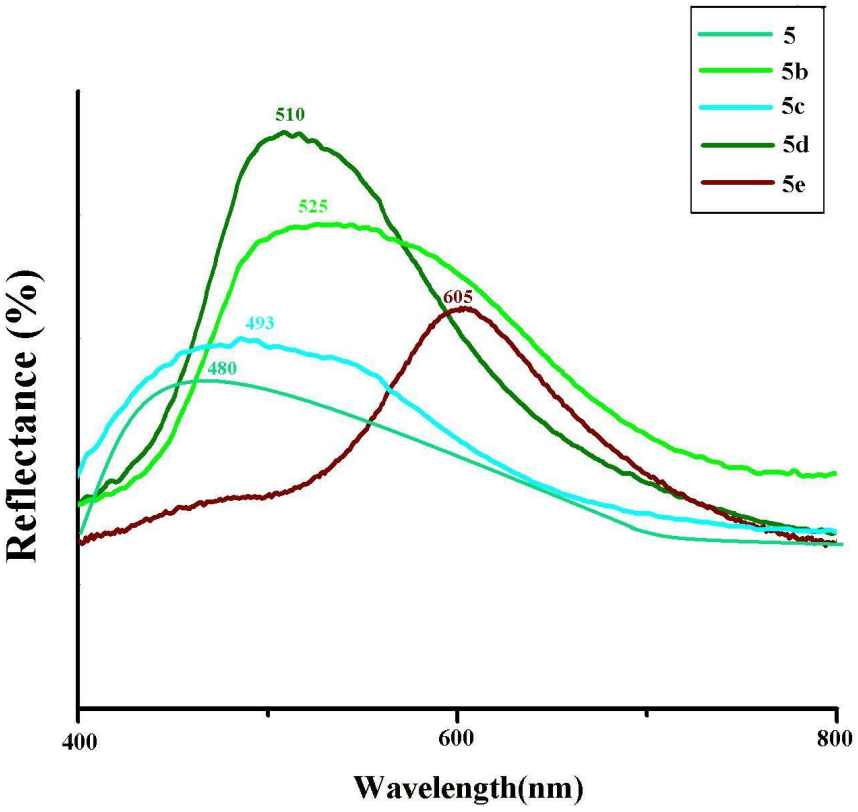


Fig. S13 The UV-vis spectra of as-synthesized **5**, **5b**, **5c**, **5d** and **5e**.

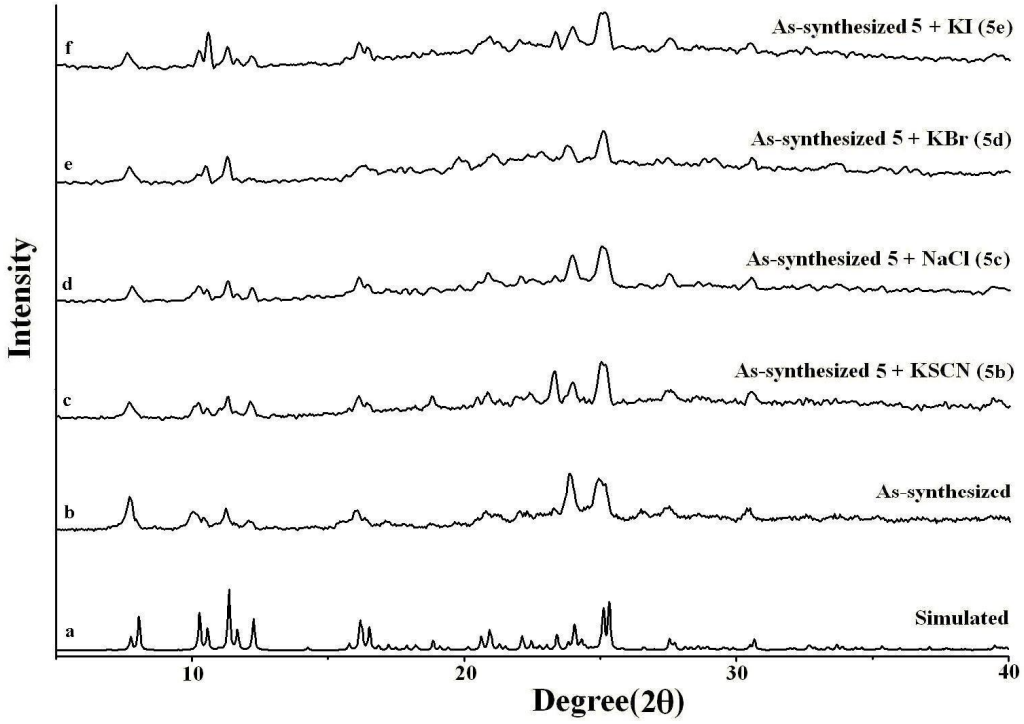


Fig. S14 The PXRD patterns of simulated from the X-ray single structure of **5** (**a**), as-synthesized **5** (**b**) and diffraction patterns obtained after immersion **5b** (**c**), **5c** (**d**), **5d** (**e**) and **5e** (**f**) in water for several days.