Electronic Supplementary Material (ESI) for Dalton Transactions.

NIR emission and luminescent sensing of lanthanide-organic framework with Lewis basic imidazole and pyridyl Sites

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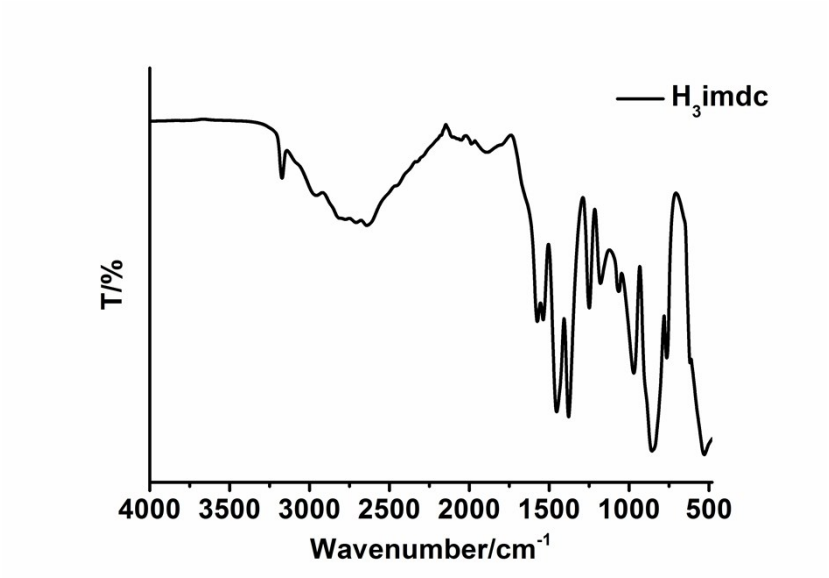

Fig. S1 IR spectrum of H_3imdc ligand.

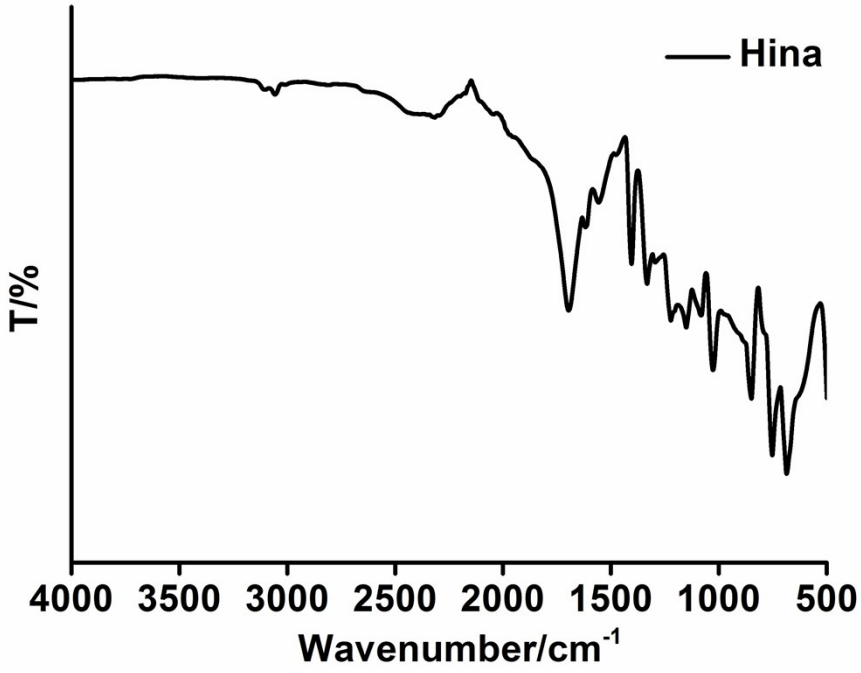

Fig. S2 IR spectrum of Hina ligand

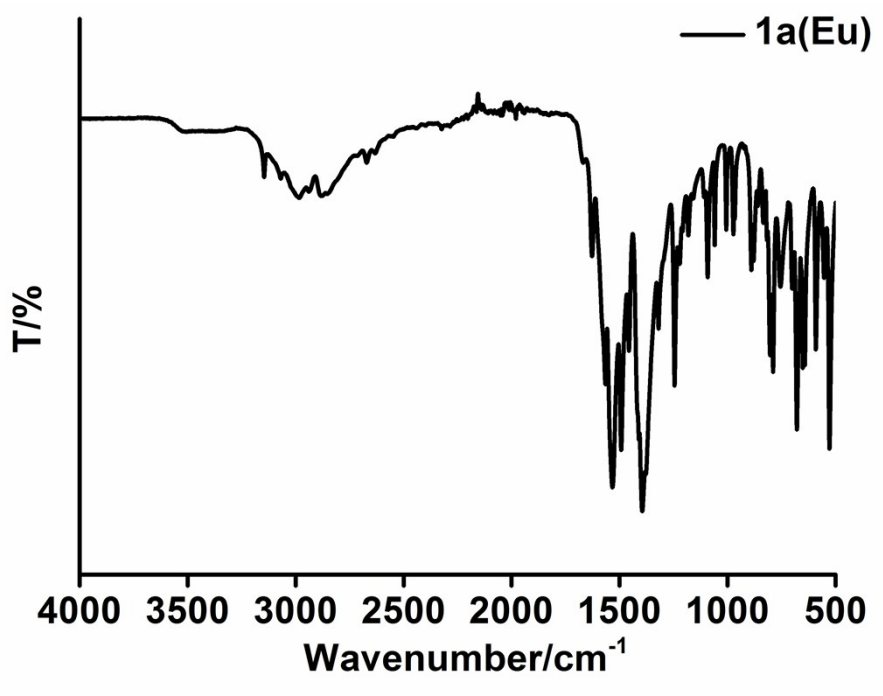

Fig. S3 IR spectra of Complex **1a** (Eu)

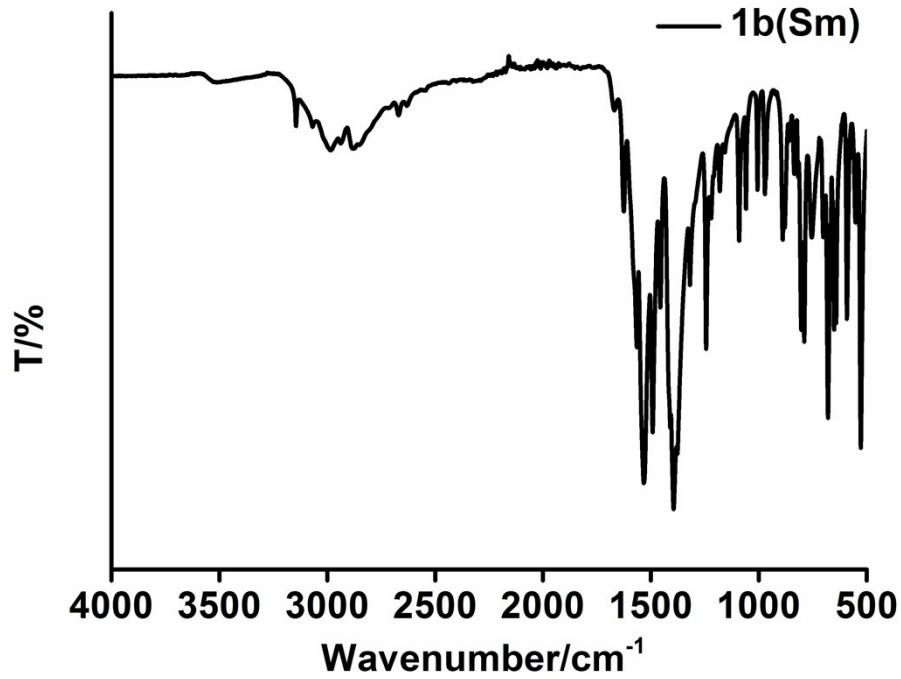

Fig. S4 IR spectra of Complex **1b**(Sm)

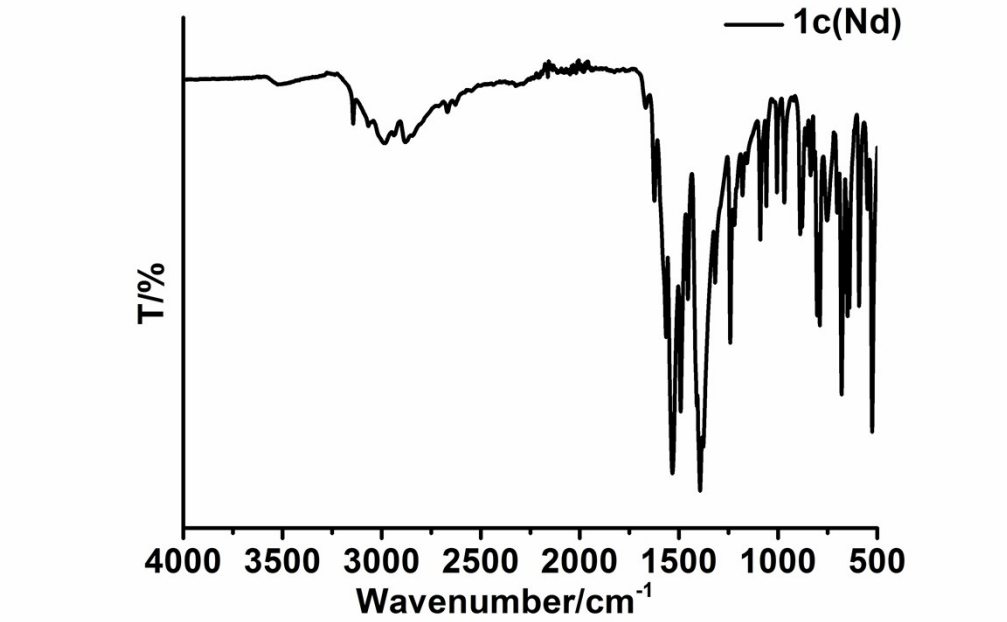

Fig. S5 IR spectra of Complex **1c** (Nd)

Table S1 Select Bond lengths [Å] and angles [°] for 1a.

Bond	Dist[Å]	Bond	Dist[Å]
Eu(1)-O(5)	2.286(3)	Eu(1)-O(1)	2.505(3)
Eu(1)-O(6)#1	2.386(3)	Eu(1)-N(1)	2.514(3)
Eu(1)-O(2)#2	2.404(3)	O(2)-Eu(1)#4	2.404(3)
Eu(1)-O(3)#2	2.434(2)	O(3)-Eu(1)#4	2.434(2)
Eu(1)-O(1W)	2.452(3)	O(4)-Eu(1)#5	2.477(2)
Eu(1)-O(4)#3	2.478(2)	O(6)-Eu(1)#1	2.386(3)

Bond	Angles(°)	Bond	Angles(°)
O(5)-Eu(1)-O(6)#1	104.53(10)	O(1W)-Eu(1)-O(1)	125.19(9)
O(5)-Eu(1)-O(2)#2	88.68(11)	O(4)#3-Eu(1)-O(1)	119.85(9)
O(6)#1-Eu(1)-O(2)#2	143.02(9)	O(5)-Eu(1)-N(1)	143.03(10)
O(5)-Eu(1)-O(3)#2	76.00(9)	O(6)#1-Eu(1)-N(1)	85.18(10)
O(6)#1-Eu(1)-O(3)#2	74.73(9)	O(2)#2-Eu(1)-N(1)	104.93(10)
O(2)#2-Eu(1)-O(3)#2	75.34(8)	O(3)#2-Eu(1)-N(1)	140.38(9)
O(5)-Eu(1)-O(1W)	75.42(10)	O(1W)-Eu(1)-N(1)	73.05(10)
O(6)#1-Eu(1)-O(1W)	74.48(9)	O(4)#3-Eu(1)-N(1)	70.97(10)
O(2)#2-Eu(1)-O(1W)	142.46(9)	O(1)-Eu(1)-N(1)	63.71(9)
O(3)#2-Eu(1)-O(1W)	130.50(9)	C(6)-O(5)-Eu(1)	176.4(3)
O(5)-Eu(1)-O(4)#3	80.98(9)	C(1)-O(1)-Eu(1)	122.5(2)
O(6)#1-Eu(1)-O(4)#3	142.52(9)	C(5)-N(1)-Eu(1)	134.3(3)
O(2)#2-Eu(1)-O(4)#3	72.90(9)	C(2)-N(1)-Eu(1)	119.0(2)

O(3)#2-Eu(1)-O(4)#3	140.86(9)	C(1)-O(2)-Eu(1)#4	151.7(2)
O(1W)-Eu(1)-O(4)#3	71.16(9)	O(3)#2-Eu(1)-O(1)	77.31(9)
O(5)-Eu(1)-O(1)	153.22(9)	C(4)-O(3)-Eu(1)#4	151.1(2)
O(6)#1-Eu(1)-O(1)	70.05(9)	C(4)-O(4)-Eu(1)#5	160.8(3)
O(2)#2-Eu(1)-O(1)	82.60(9)	C(6)-O(6)-Eu(1)#1	131.6(3)

Table. S2 H-Bonds of compound 1a

Donor	H....Acceptor	D - H (Å)	H...A(Å)	D...A(Å)	D - H…A(°)
N2	H2 O2	0.86	1.96	2.798(4)	163
O1W	H1WB N3	0.85	1.93	2.770(5)	168

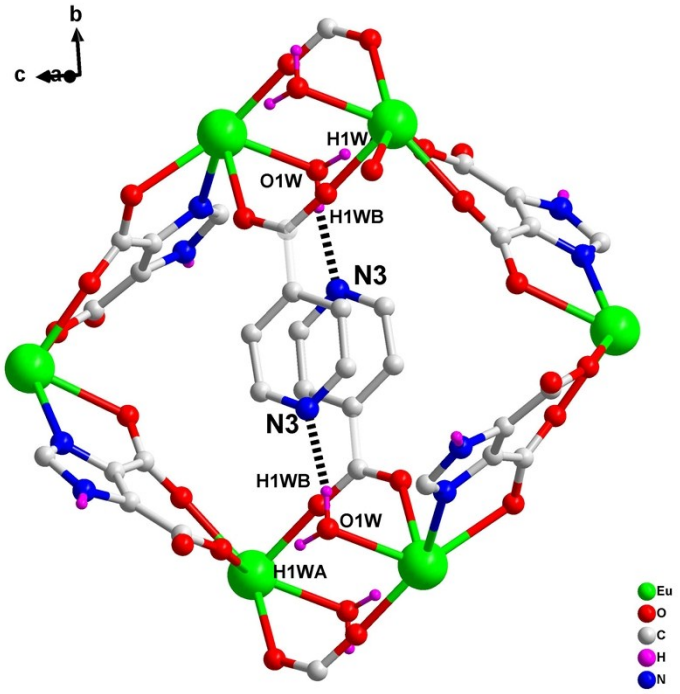

Fig. S6 Hydrogen bonds between pyridyl groups and coordinated water molecules in compound **1a**

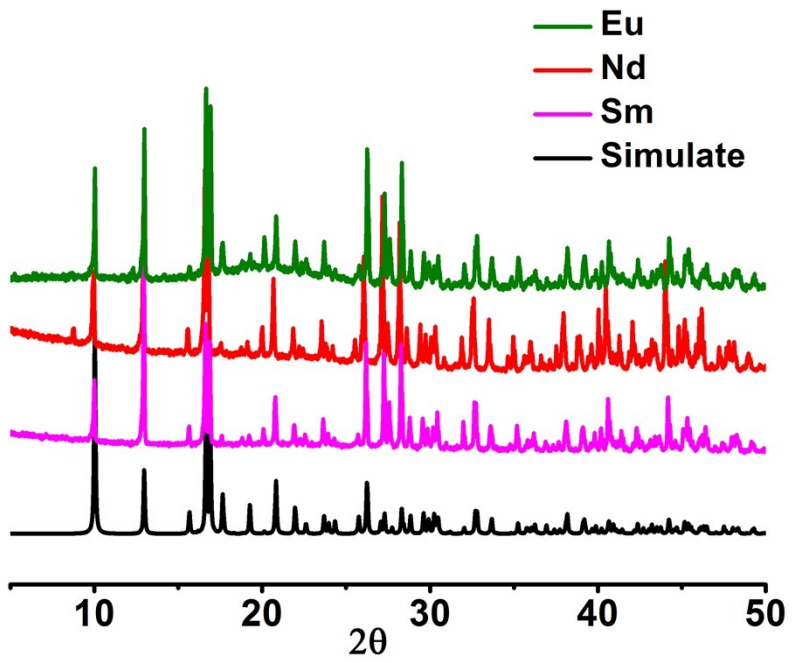

Fig. S7 Powder XRD patterns of **1a**(Eu), **1b**(Sm) and **1c**(Nd)

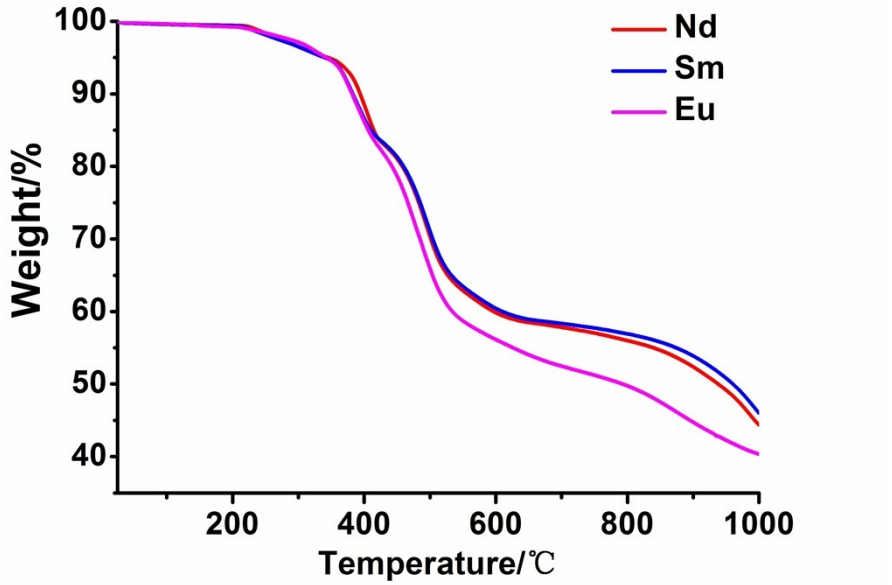

Fig. S8 The TGA diagrams of complexes **1a**(Eu), **1b**(Sm) and **1c**(Nd).

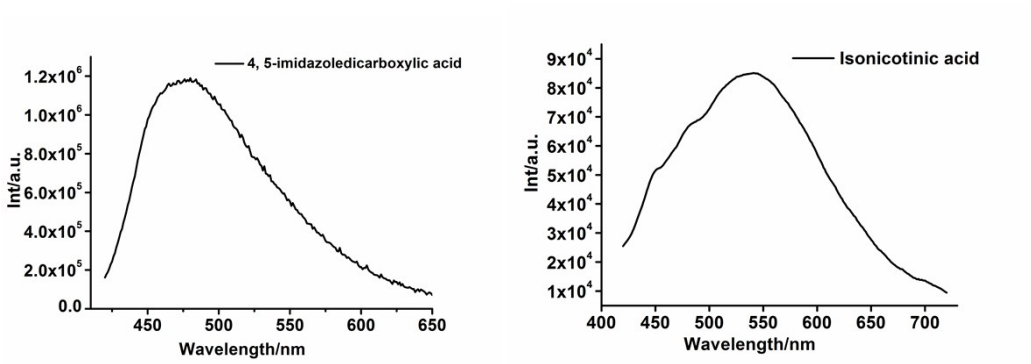

Fig S9. The emission spectra of 4, 5-imidazoledicarboxylic acid and isonicotinic acid ligands

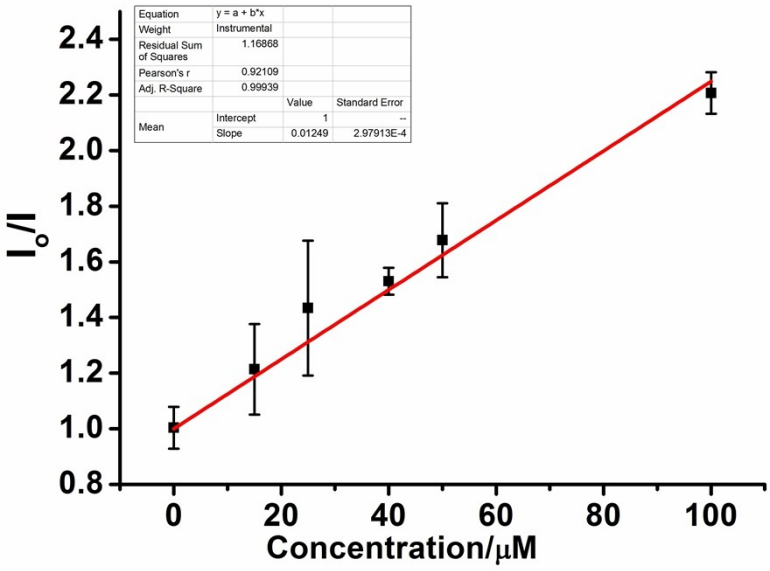

Fig. S10 Stern-Volmer curves for **1a** when exposed to 10^{-3}mol/L Fe^{3+}.

Table S3 Comparison of K(SV) values and limit of detection in Ln-MOFs

Ln-MOF luminescent materials	**substrates**	**Detection limit/(mol/L)**	**KSv m^{-1}**	**ref**
$[Eu(HL)(H_2O)_2]_n \cdot 2H_2O$	Fe^{3+}	10^{-6}	------	16
$\{[Eu(L)(BPDC)1/2(NO_3)]\cdot H_3O\}_n$	Fe^{3+}	5×10^{-7}	5.16×10^4	21
Eu_4L_3	Fe^{3+}	10^{-5}	2942	41
Eu-1,4-NDC	Fe^{3+}	10^{-6}	9340	42
Our work	Fe^{3+}	10^{-5}	13000	
Eu_4L_3	$Cr_2O_7^{2-}$	10^{-5}	1526	41
Eu-1,4-NDC	$Cr_2O_7^{2-}$	10^{-6}	11150	42
Our work	$Cr_2O_7^{2-}$	10^{-5}	2462	

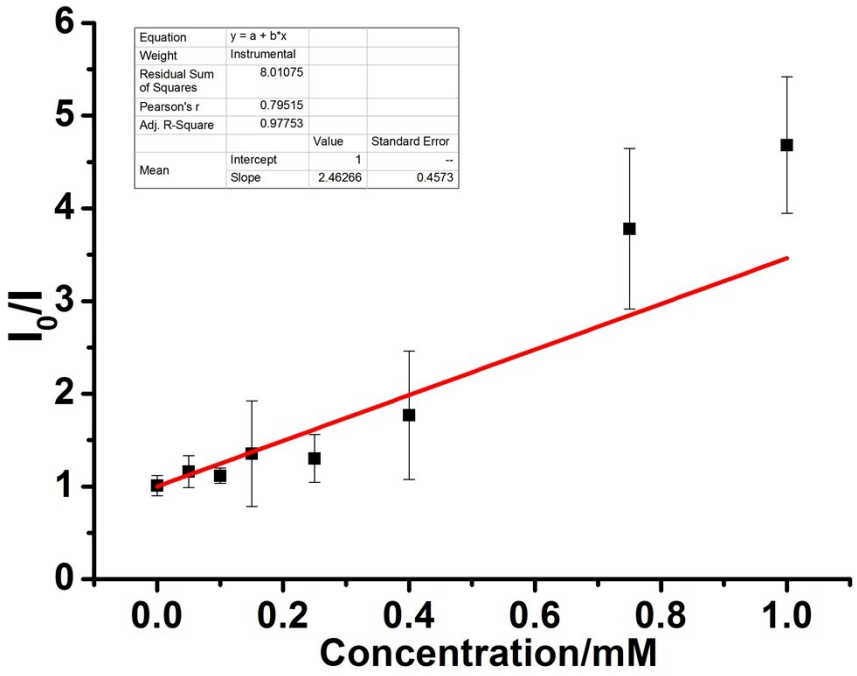

Fig. S11 Stern-Volmer curves for **1a** when exposed to 10^{-2} mol/L $Cr_2O_7^{2-}$.

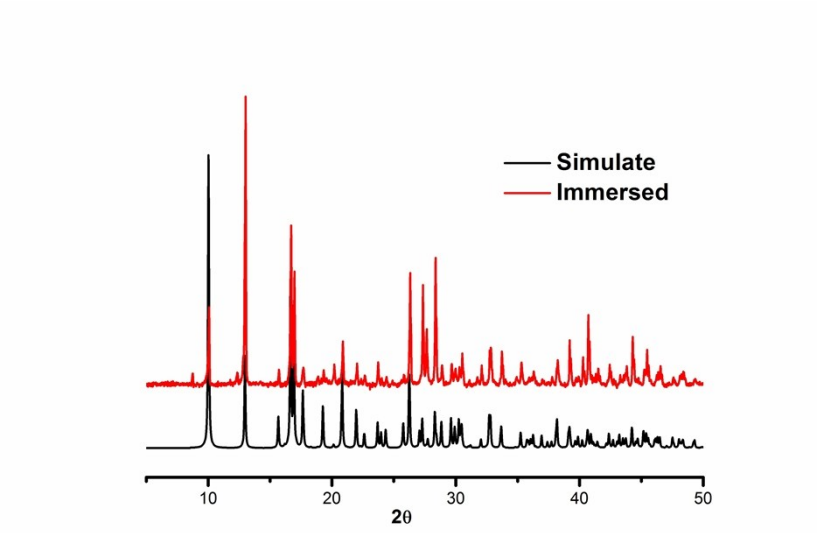

Fig. S12 The PXRD of complexes **1a** after treated with Fe^{3+} for 1 hours.

Table S4 The ICP results of complexes 1 after treated with Fe^{3+} for 12 hours.

	μM
Initial value/Fe^{3+}	0.75
After treated with Fe^{3+} for 6 hours	0.32

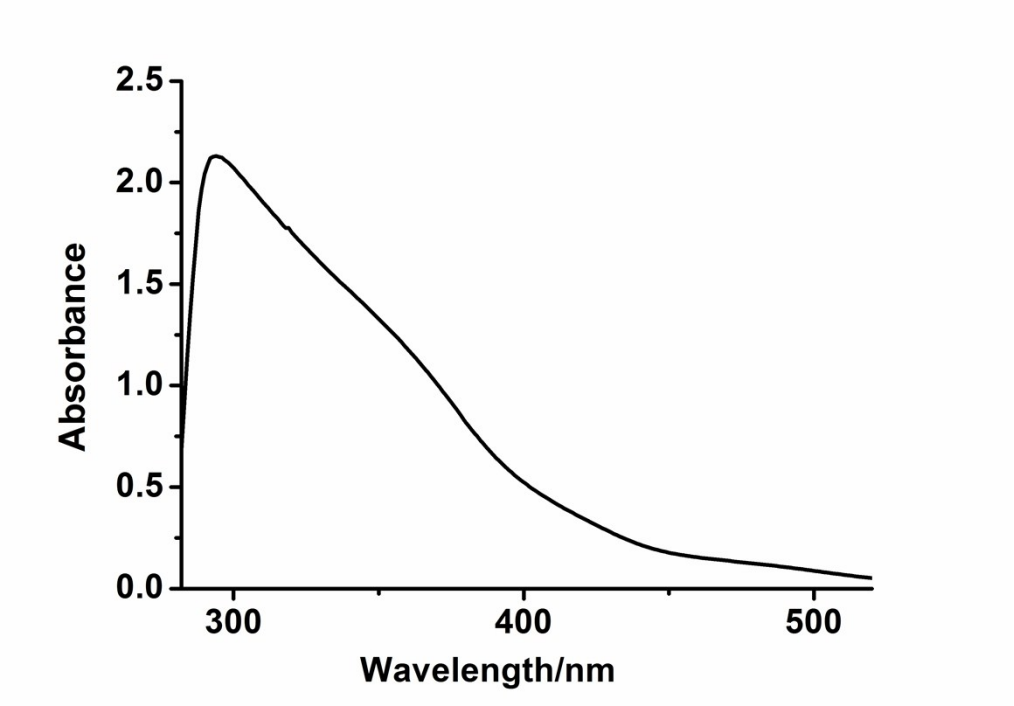

Fig. S13 The UV-Vis spectra of aqueous solution containing $FeCl_3$.

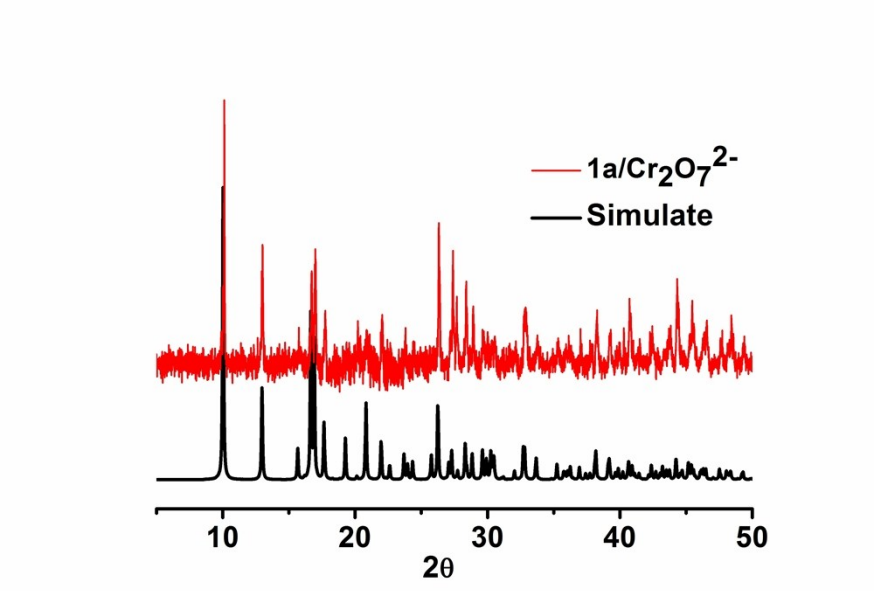

Fig. S14 The PXRD of complexes **1a** after treated with $Cr_2O_7^{2-}$ for 1 hours.

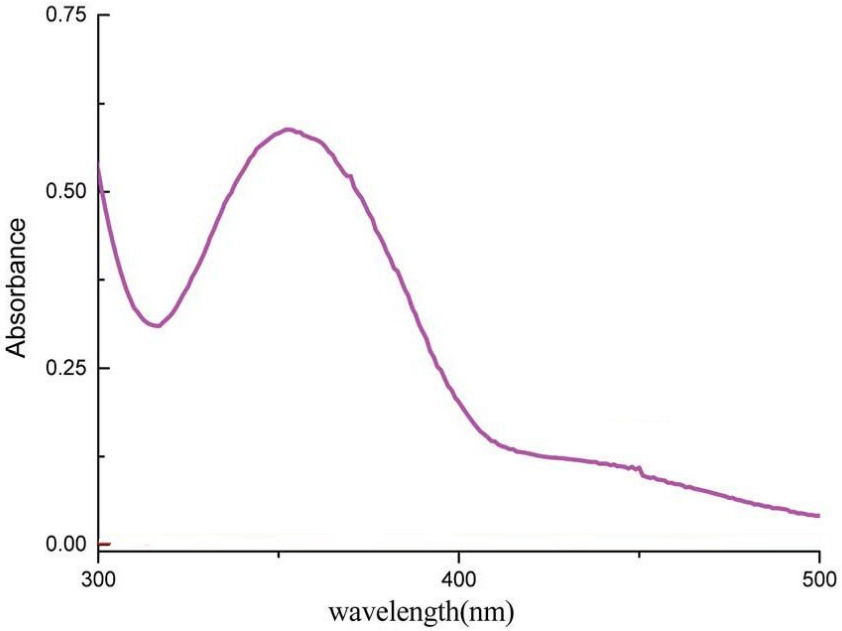

Fig. S15 The UV-Vis spectra of $K_2Cr_2O_7$.