Effects of solvents and metal ions on the synthesis, structural diversity and magnetic properties of 5'-nitro-[1,1':3',1''-terphenyl]-3,3'',5,5''-tetracarboxylic acid ligand and a highly sensitive sensor for Fe^{3+}

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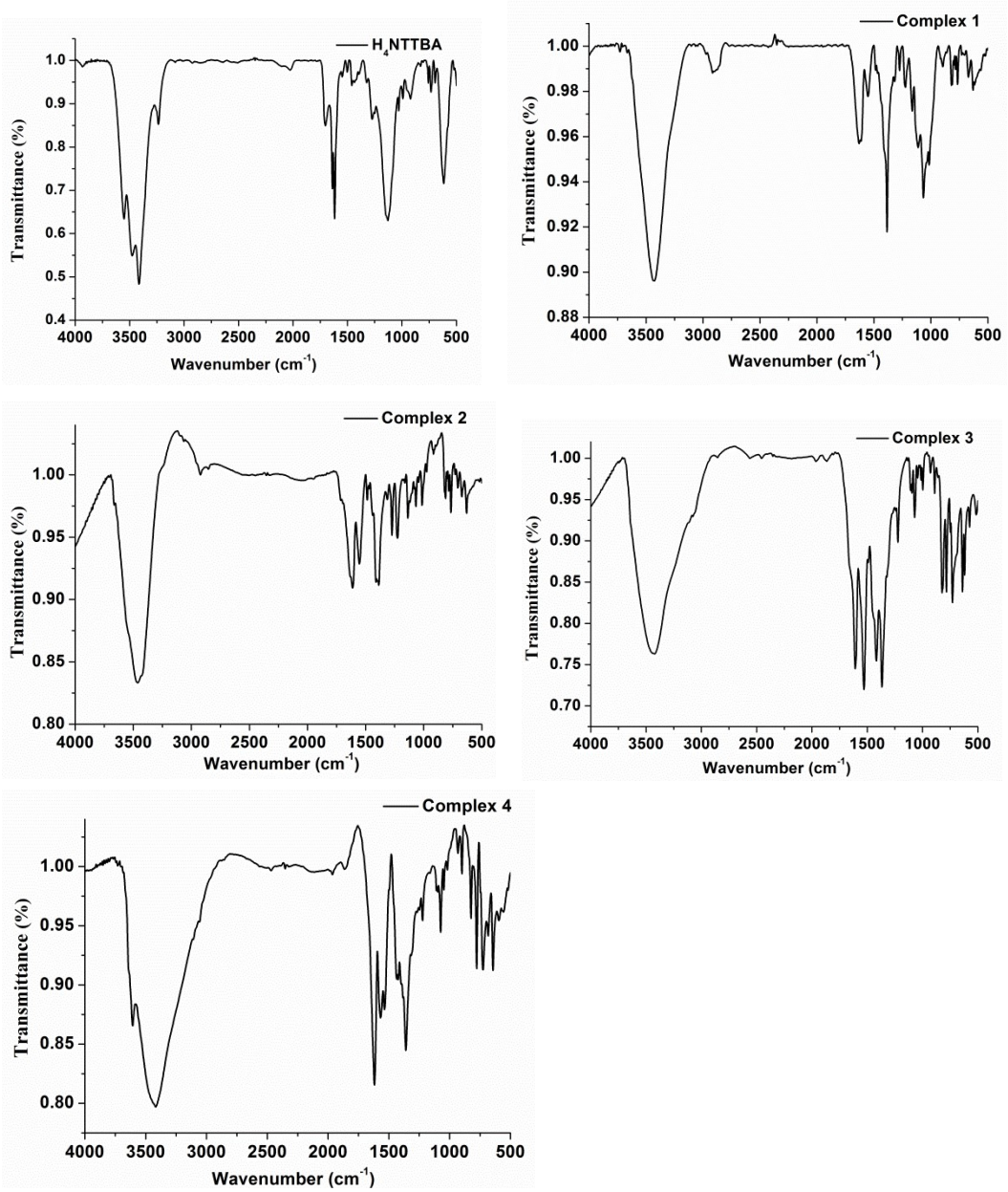

Fig. S1 The IR spectra of H_4nttba ligand and complexes **1**-**4**.

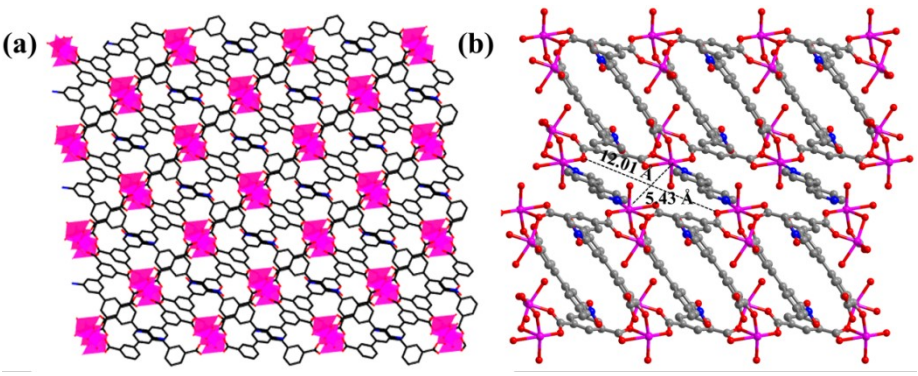

Fig. S2 (a) View of the single 2D framework of complex **1**. (b) The void size of the 2D

framework of complex **1**.

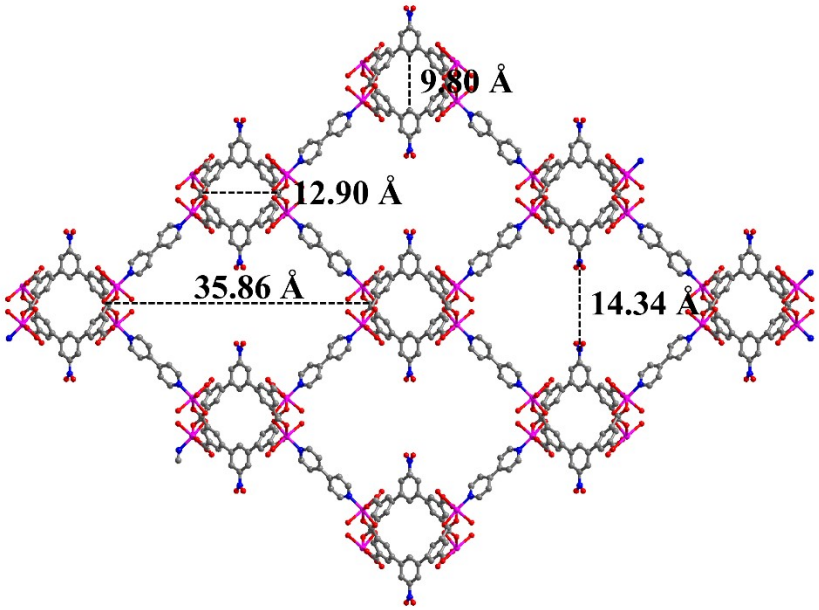

Fig. S3 The void size of the 2D framework of complex **2**.

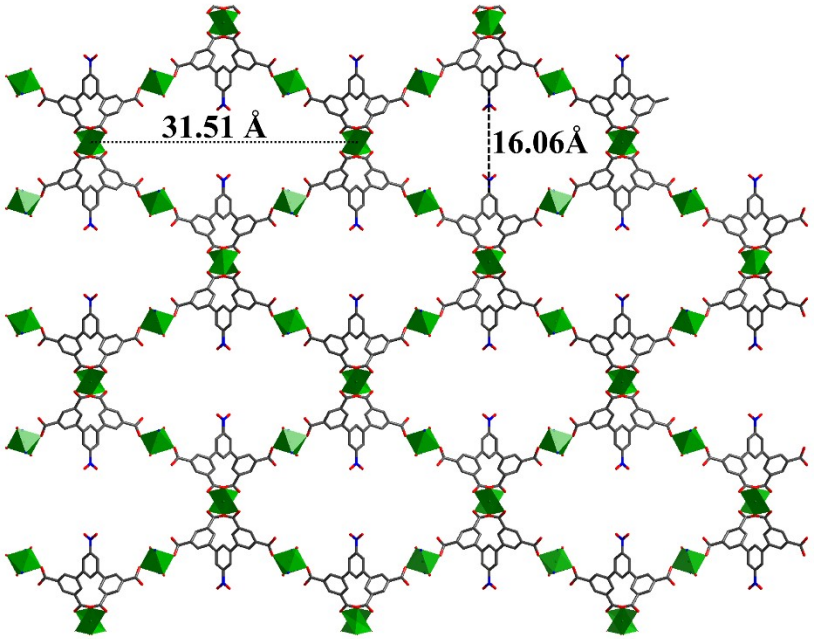

Fig. S4 The void size of the 2D framework of complex **3**.

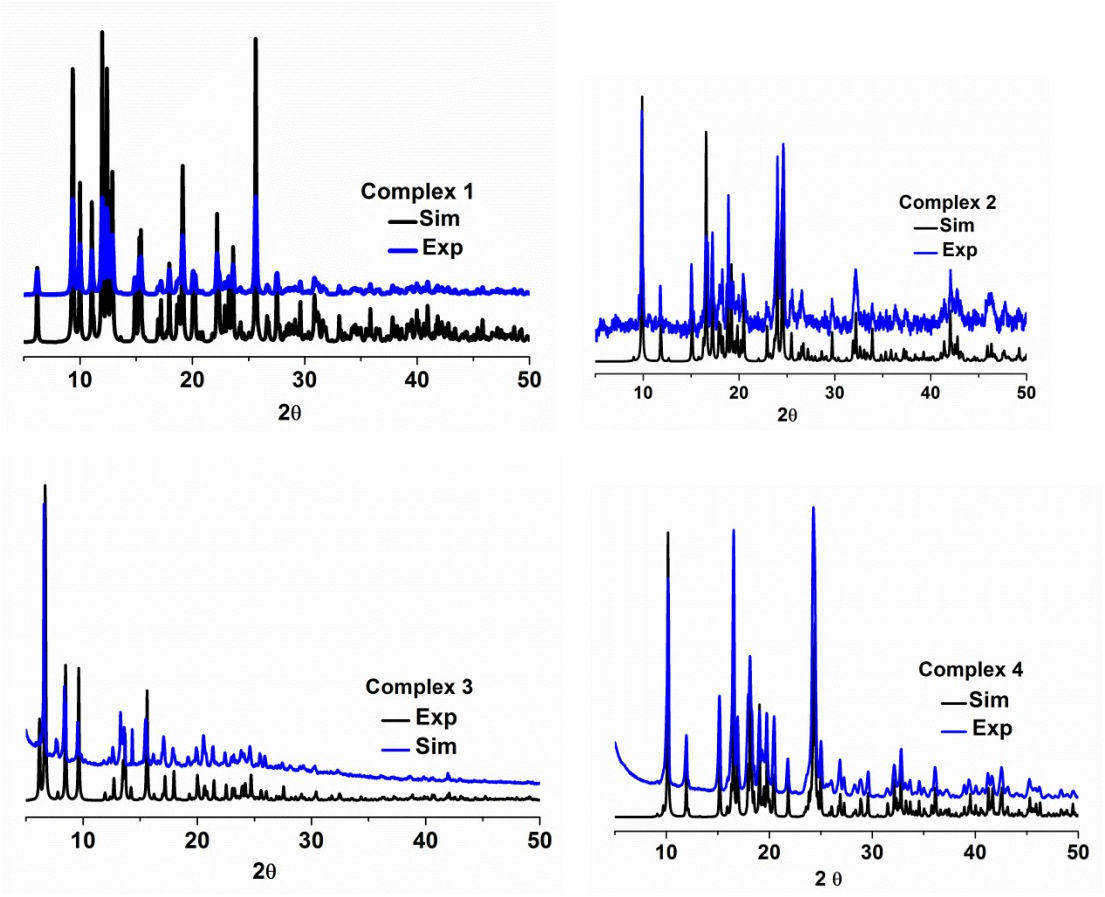

Fig. S5 PXRD patterns of complexes **1**–**4** at room temperature. Blue patterns correspond to the experimental data obtained using the as synthesized bulk samples. Black patterns were simulated from the single crystal X-ray data.

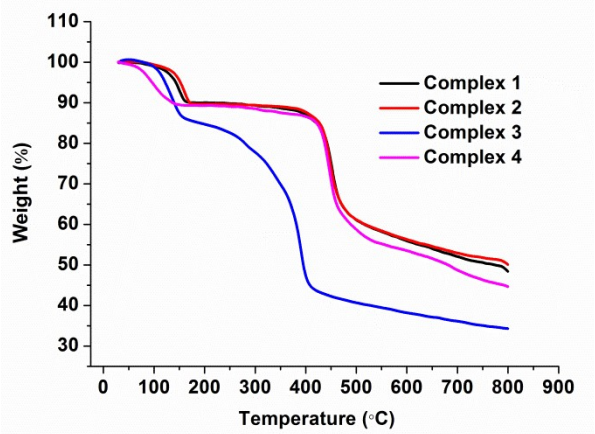

Fig. S6 The thermal curves of complexes **1**-**4**.

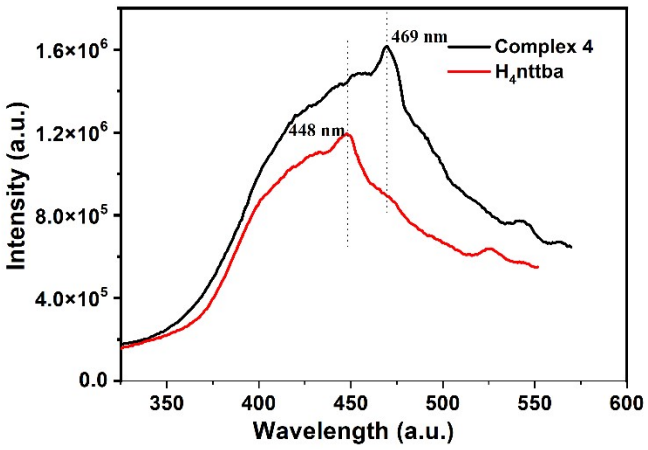

Fig. S7 The solid-state emission spectra of complex **4** and H_4nttba at room temperature.

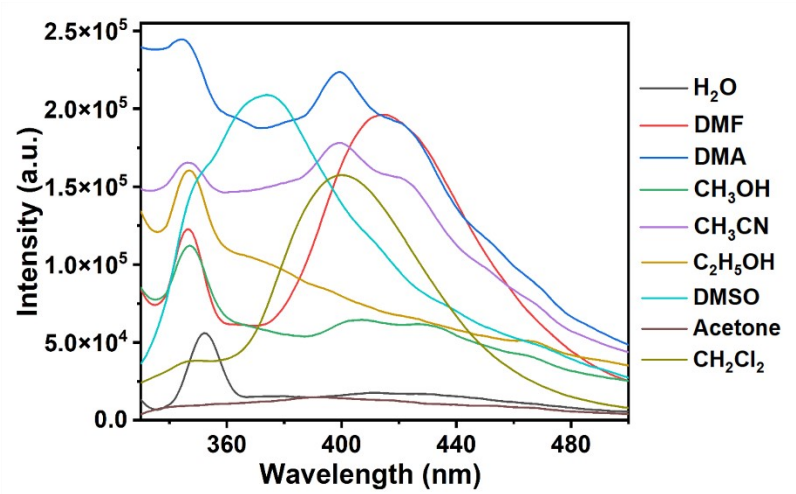

Fig.S8 The emission spectra of complex **4** in different solvents.

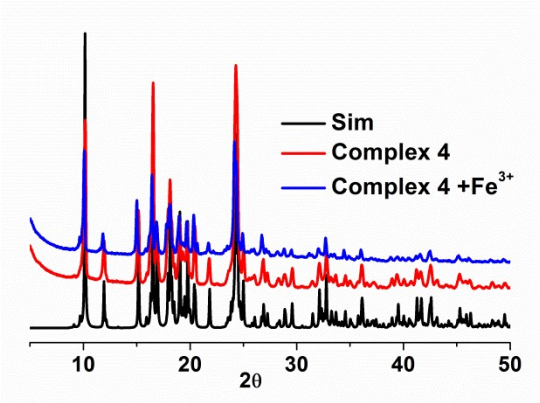

Fig. S9 The PXRD patterns of simulated complex **4**, the PXRD patterns of 4 for the recognition of Fe^{3+} after five recycling processes.

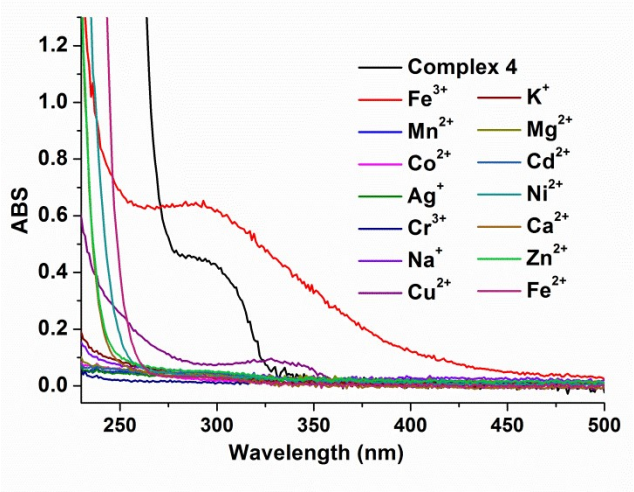

Fig. S10 Liquid U‐*vis* spectra of complex **4** , Fe^{3+} in the solution.

Table S1 Selected bond distances (Å) and angles (°) for **1, 2, 3** and **4**.

Complex **1**			
Co1—O8^{i}	2.050 (3)	Co2—O7	1.896 (3)
Co1—N2	2.084 (3)	Co2—O1^{iii}	1.954 (3)
Co1—O3^{ii}	2.086 (3)	Co2—O4^{iv}	1.963 (3)
Co1—O11	2.134 (3)	Co2—O9^{v}	2.124 (3)
Co1—O9	2.165 (3)	Co2—O12	2.262 (7)
Co1—O10	2.258 (3)		
O8^{i}—Co1—N2	95.94 (12)	O3^{ii}—Co1—O11	168.71 (13)
O8^{i}—Co1—O3^{ii}	105.73 (13)	O8^{i}—Co1—O9	100.32 (10)
N2—Co1—O3^{ii}	88.61 (12)	N2—Co1—O9	163.65 (11)
O8^{i}—Co1—O11	85.56 (13)	O3^{ii}—Co1—O9	88.67 (11)
N2—Co1—O11	90.60 (12)	O11—Co1—O9	88.93 (12)
O8^{i}—Co1—O10	157.31 (11)	O7—Co2—O1^{iii}	108.91 (15)
N2—Co1—O10	104.59 (11)	O7—Co2—O4^{iv}	124.15 (17)
O3^{ii}—Co1—O10	84.62 (12)	O1^{iii}—Co2—O4^{iv}	120.64 (15)
O11—Co1—O10	84.69 (12)	O7—Co2—O9^{v}	92.97 (13)
O9—Co1—O10	59.10 (9)	O1^{iii}—Co2—O9^{v}	111.61 (14)
O4^{iv}—Co2—O9^{v}	91.56 (13)	O4^{iv}—Co2—O12	81.3 (2)
O7—Co2—O12	74.5 (2)	O9^{v}—Co2—O12	158.1 (3)
O1^{iii}—Co2—O12	89.7 (3)		

Complex **2**			
Co1—O1	2.021 (2)	Co1—O7	2.121 (3)
Co1—O4^{i}	2.060 (3)	Co1—O6	2.162 (3)
Co1—N2	2.067 (3)	Co1—O3^{i}	2.277 (3)
O1—Co1—O4^{i}	95.50 (11)	O1—Co1—O6	87.16 (12)
O1—Co1—N2	98.42 (12)	O4^{i}—Co1—O6	91.09 (13)
O4^{i}—Co1—N2	165.92 (12)	N2—Co1—O6	87.50 (13)
O1—Co1—O7	92.83 (11)	O7—Co1—O6	177.68 (12)
O4^{i}—Co1—O7	91.22 (13)	O1—Co1—O3^{i}	155.38 (11)
N2—Co1—O7	90.21 (13)	O4^{i}—Co1—O3^{i}	60.47 (10)
N2—Co1—O3^{i}	105.46 (11)	O6—Co1—O3^{i}	87.97 (12)
O7—Co1—O3^{i}	92.98 (12)		
Complex **3**			
Ni1—O6^{i}	2.0484 (12)	Ni2—N1^{ii}	2.0537 (15)
Ni1—O6	2.0485 (12)	Ni2—N1^{iii}	2.0537 (15)
Ni1—O4	2.0705 (11)	Ni2—O2	2.0943 (12)
Ni1—O4^{i}	2.0705 (11)	Ni2—O2^{iv}	2.0944 (12)
Ni1—N2	2.1219 (14)	Ni2—O1^{iv}	2.1283 (13)
Ni1—N2^{i}	2.1220 (14)	Ni2—O1	2.1284 (13)
O6^{i}—Ni1—O6	180.0	O4—Ni1—O4^{i}	180.00 (6)
O6^{i}—Ni1—O4	87.87 (5)	O6^{i}—Ni1—N2	90.21 (5)
O6—Ni1—O4	92.13 (5)	O6—Ni1—N2	89.79 (5)
O6^{i}—Ni1—O4^{i}	92.14 (5)	O4—Ni1—N2	89.33 (5)
O6—Ni1—O4^{i}	87.87 (5)	O4^{i}—Ni1—N2	90.67 (5)
O6^{i}—Ni1—N2^{i}	89.79 (5)	N1^{ii}—Ni2—O2	96.21 (6)
O6—Ni1—N2^{i}	90.21 (5)	N1^{iii}—Ni2—O2	100.67 (5)
O4—Ni1—N2^{i}	90.68 (5)	N1^{ii}—Ni2—O2^{iv}	100.67 (5)
O4^{i}—Ni1—N2^{i}	89.32 (5)	N1^{iii}—Ni2—O2^{iv}	96.21 (6)
N2—Ni1—N2^{i}	180.0	O2—Ni2—O2^{iv}	156.16 (7)
N1^{ii}—Ni2—N1^{iii}	89.51 (9)	N1^{ii}—Ni2—O1^{iv}	162.90 (5)
N1^{iii}—Ni2—O1^{iv}	92.15 (6)	N1^{iii}—Ni2—O1	162.90 (5)

O2—Ni2—O1^{iv}	100.20 (5)	O2—Ni2—O1	62.23 (5)
O2^{iv}—Ni2—O1^{iv}	62.23 (5)	O2^{iv}—Ni2—O1	100.20 (5)
N1^{ii}—Ni2—O1	92.15 (6)	O1^{iv}—Ni2—O1	91.25 (8)
Complex **4**			
Zn1—O4^{i}	1.948 (3)	Zn1—O6	2.156 (4)
Zn1—O2	1.966 (3)	Zn1—O7	2.248 (4)
Zn1—N2	2.020 (3)		
O4^{i}—Zn1—O2	104.06 (15)	O4^{i}—Zn1—O7	89.34 (16)
O4^{i}—Zn1—N2	149.22 (15)	O2—Zn1—O7	88.22 (15)
O2—Zn1—N2	106.04 (15)	N2—Zn1—O7	85.34 (15)
O4^{i}—Zn1—O6	92.81 (17)	O6—Zn1—O7	175.61 (15)
O2—Zn1—O6	94.96 (14)	N2—Zn1—O6	90.86 (15)

Table S2. A comparison of selected MOFs-based luminescent sensors for the detection of Fe^{3+} ion.

MOFsand related materials	Analyte	$K_{sv}(M^{-1})$	Detection Limit (mol/L)	Ref
Eu^{3+}@MIL-124	Fe^{3+}	3.874×10^{4}	2.8×10^{-7}	S1
NTU-9-NS(Ti)	Fe^{3+}	-	4.5×10^{-7}	S2
$[Cd_2(L)(bimid)(DMF)_2]\cdot(DMF)$	Fe^{3+}	3.75×10^{4}	3.70×10^{-7}	S3
Eu−BPDA	Fe^{3+}	1.25×10^{4}	9×10^{-7}	S4
$\{Cd_3\cdot L^{6}\cdot(BTB)_2\cdot 2DMF\}_n$	Fe^{3+}	1.01×10^{4}	1.12×10^{-6}	S5
$Eu_2(OH\text{-}BDC)_3$	Fe^{3+}	-	1.17×10^{-6}	S6
$\{[Cd(L)_{0.5})(1,8\text{-}NDC)\cdot H_2O]\}_n$	Fe^{3+}	7.75×10^{3}	1.40×10^{-6}	S7
[Zn(L)(bpe)]·DMF	Fe^{3+}	2.27×10^{4}	1.55×10^{-6}	S8
BUT-14	Fe^{3+}	2.17×10^{3}	3.8×10^{-6}	S9
$[Zn_2(cptpy)(btc)(H_2O)]_n$	Fe^{3+}	5.456×10^{3}	4.33×10^{-6}	S10
$\{[Zn(NTTBA)_{0.5}(4,4'bpy)_{0.5}(H_2O)_2]\cdot 0.5H_2O\}_n$	Fe^{3+}	5.05×10^{3}	6.96×10^{-6}	This work
$[Tb(BTB)(DMF)]\cdot 1.5DMF\cdot 2.5H_2O$	Fe^{3+}	-	1×10^{-5}	S11
$\{[Zn_2(BIBP)_2(HL)_2]\cdot 2H_2O\}_n$	Fe^{3+}	2.21×10^{4}	2.29×10^{-5}	S12
FJI-C8 (Zn)	Fe^{3+}	8245	2.33×10^{-5}	S13
$[Cd(Hcbic)]_n$	Fe^{3+}	1.8×10^{5}	3.1×10^{-5}	S14
$[Eu(atpt)_{1.5}(phen)(H_2O)]_n$	Fe^{3+}	7.60×10^{3}	4.5×10^{-5}	S15
$\{[Zn(L^{1})(dcdps)]\}_n$	Fe^{3+}	7.004×10^{3}	6.21×10^{-5}	S16
$\{Zn(L^{1})(bdc)\}_n$	Fe^{3+}	9.066×10^{3}	4.45×10^{-5}	S16

$[Zn_5(hfipbb)_4(trz)_2(H_2O)_2]$	Fe^{3+}	4.1×10^5	1.8×10^{-4}	S17
$[Ln(\mu_3\text{-cpta})(phen)(H_2O)_2]n$	Fe^{3+}	2138	2.0×10^{-4}	S18
HPU-1 (Zn)	Fe^{3+}	1.0×10^4	1.09×10^{-3}	S19

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