Electronic Supplementary Information (ESI)

Three 3D Lanthanide-Organic Frameworks with sra Topology: Syntheses, Structures, Luminescence and Magnetic Properties

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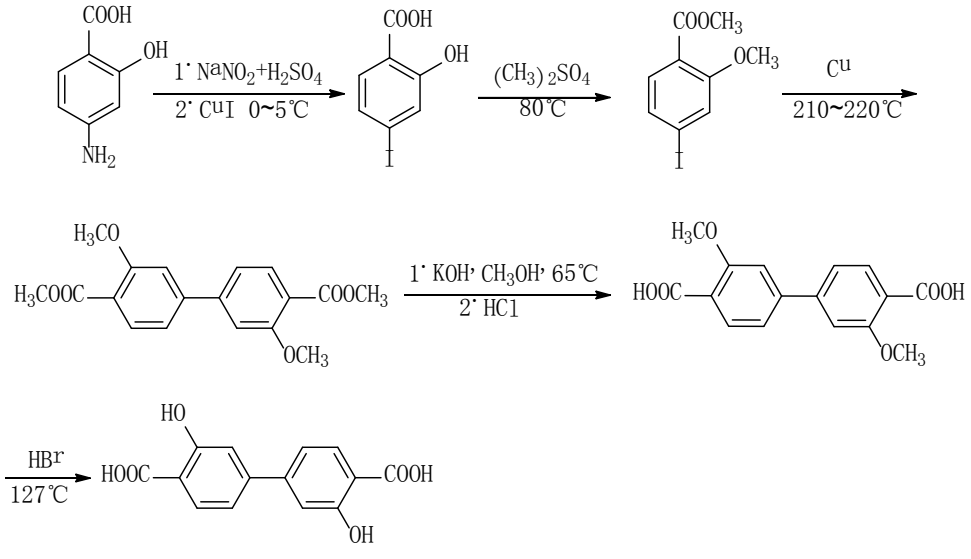

Scheme S1 Synthesis of 3,3′-dihydroxy-4,4′-biphenyldicarboxylic acid (H_4L)

Table S1 Selected bond lengths (Å) for LOFs **1**–**3**

		1	
Eu1–O1	2.764(5)	Eu1–O2	2.416(5)
Eu1–O7	2.372(6)	Eu1–O3^{i}	2.387(5)
Eu1–O1^{ii}	2.384(5)	Eu1–O2^{iii}	2.359(5)
Eu1–O5^{iii}	2.215(5)	Eu1–O4^{iv}	2.397(5)
Eu1···Eu1^{iii}	3.914(5)	Eu1···Eu1^{ii}	4.142(5)
		2	
Gd1–O1	2.773(6)	Gd1–O2	2.424(5)
Gd1–O7	2.348(7)	Gd1–O3^{i}	2.363(6)
Gd1–O1^{ii}	2.371(6)	Gd1–O2^{iii}	2.343(6)
Gd1–O5^{iii}	2.216(6)	Gd1–O4^{iv}	2.385(6)
Gd1···Gd1^{iii}	3.891(6)	Gd1···Gd1^{ii}	4.136(6)
		3	
Dy1–O1	2.716(6)	Dy1–O2	2.371(6)
Dy1–O7	2.336(7)	Dy1–O3^{i}	2.343(7)
Dy1–O1^{ii}	2.344(6)	Dy1–O2^{iii}	2.326(6)
Dy1–O5^{iii}	2.190(6)	Dy1–O4^{iv}	2.357(6)
Dy1···Dy1^{iii}	3.830(6)	Dy1···Dy1^{ii}	4.061(6)

Symmetry codes: (i) 3–*x*, *y*+1/2, –*z*–1/2; (ii) 2–*x*, –*y*, –*z*; (iii) 3–*x*, –*y*, –*z*; (iv) *x*, –*y*–1/2, *z*+1/2.

Table S2 Selected bond angles (°) for LOFs **1**–**3**

			1		
O1–Eu1–O2	49.09(16)	O1–Eu1–O7	87.60(2)	O1–Eu1–O3^{i}	75.86(18)
O1–Eu1–O1^{ii}	73.09(18)	O1–Eu1–O2^{iii}	117.28(16)	O1–Eu1–O5^{iii}	171.27(17)
O1–Eu1–O4^{iv}	95.52(18)	O2–Eu1–O7	132.10(2)	O2–Eu1–O3^{i}	73.35(19)
O1^{ii}–Eu1–O2	104.32(17)	O2–Eu1–O2^{iii}	69.90(2)	O2–Eu1–O5^{iii}	138.88(19)
O2–Eu1–O4^{iv}	71.12(19)	O3^{i}–Eu1–O7	77.20(2)	O1^{ii}–Eu1–O7	75.20(2)
O2^{iii}–Eu1–O7	135.10(2)	O5^{iii}–Eu1–O7	86.20(2)	O4^{iv}–Eu1–O7	143.40(2)
O1^{ii}–Eu1–O3^{i}	138.88(18)	O2^{iii}–Eu1–O3^{i}	74.17(19)	O3^{i}–Eu1–O5^{iii}	108.7(2)
O3^{i}–Eu1–O4^{iv}	138.88(19)	O1^{ii}–Eu1–O2^{iii}	145.05(19)	O1^{ii}–Eu1–O5^{iii}	99.33(19)
O1^{ii}–Eu1–O4^{iv}	70.98(19)	O2^{iii}–Eu1–O5^{iii}	71.41(18)	O2^{iii}–Eu1–O4^{iv}	74.71(18)
O4^{iv}–Eu1–O5^{iii}	85.80(2)	Eu1–O1–Eu1^{ii}	106.90(2)	Eu1–O2–Eu1^{iii}	110.09(2)
			2		
O1–Gd1–O2	49.03(18)	O1–Gd1–O7	88.00(2)	O1–Gd1–O3^{i}	76.24(19)
O1–Gd1–O1^{ii}	73.20(2)	O1–Gd1–O2^{iii}	117.78(18)	O1–Gd1–O5^{iii}	170.35(19)
O1–Gd1–O4^{iv}	96.30(2)	O2–Gd1–O7	132. 70(2)	O2–Gd1–O3^{i}	74.10(2)
O1^{ii}–Gd1–O2	104.30(2)	O2–Gd1–O2^{iii}	70.60(2)	O2–Gd1–O5^{iii}	139.60(2)
O2–Gd1–O4^{iv}	71.60(2)	O3^{i}–Gd1–O7	77.60(2)	O1^{ii}–Gd1–O7	74.50(2)
O2^{iii}–Gd1–O7	134.90(2)	O5^{iii}–Gd1–O7	85.40(2)	O4^{iv}–Gd1–O7	142.50(2)
O1^{ii}–Gd1–O3^{i}	138.90(2)	O2^{iii}–Gd1–O3^{i}	74.20(2)	O3^{i}–Gd1–O5^{iii}	109.00(2)
O3^{i}–Gd1–O4^{iv}	139.60(2)	O1^{ii}–Gd1–O2^{iii}	145.40(2)	O1^{ii}–Gd1–O5^{iii}	98.20(2)

O1^{ii}–Gd1–O4^{iv}	71.30(2)	O2^{iii}–Gd1–O5^{iii}	71.80(2)	O2^{iii}–Gd1–O4^{iv}	74.80(2)
O4^{iv}–Gd1–O5^{iii}	84.90(2)	Gd1–O1–Gd1^{ii}	106.81(2)	Gd1–O2–Gd1^{iii}	109.39(2)
		3			
O1–Dy1–O2	50.06(19)	O1–Dy1–O7	86.40(2)	O1–Dy1–O3^{i}	74.60(2)
O1–Dy1–O1^{ii}	73.50(2)	O1–Dy1–O2^{iii}	118.00(2)	O1–Dy1–O5^{iii}	169.00(2)
O1–Dy1–O4^{iv}	98.80(2)	O2–Dy1–O7	133.00(2)	O2–Dy1–O3^{i}	75.20(2)
O1^{ii}–Dy1–O2	102.90(2)	O2–Dy1–O2^{iii}	70.70(2)	O2–Dy1–O5^{iii}	140.30(2)
O2–Dy1–O4^{iv}	71.60(2)	O3^{i}–Dy1–O7	76.80(2)	O1^{ii}–Dy1–O7	75.40(2)
O2^{iii}–Dy1–O7	134.50(2)	O5^{iii}–Dy1–O7	84.80(3)	O4^{iv}–Dy1–O7	142.40(2)
O1^{ii}–Dy1–O3^{i}	138.50(2)	O2^{iii}–Dy1–O3^{i}	74.30(2)	O3^{i}–Dy1–O5^{iii}	109.50(2)
O3^{i}–Dy1–O4^{iv}	140.50(2)	O1^{ii}–Dy1–O2^{iii}	145.30(2)	O1^{ii}–Dy1–O5^{iii}	98.00(2)
O1^{ii}–Dy1–O4^{iv}	70.60(2)	O2^{iii}–Dy1–O5^{iii}	72.90(2)	O2^{iii}–Dy1–O4^{iv}	75.10(2)
O4^{iv}–Dy1–O5^{iii}	84.40(3)	Dy1–O1–Dy1^{ii}	106.56(2)	Dy1–O2–Dy1^{iii}	109.29(2)

Symmetry codes: (i) 3–*x*, *y*+1/2, –*z*–1/2; (ii) 2–*x*, –*y*, –*z*; (iii) 3–*x*, –*y*, –*z*; (iv) *x*, –*y*–1/2, *z*+1/2.

Table S3 Hydrogen-bonding geometry (Å, °) for LOF **2**

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
O6–H6B···O4	0.82	1.90	2.609(6)	144
O6–H6B···O1^{v}	0.82	2.60	3.276(6)	141
C15–H15A···O3^{i}	0.93	2.52	3.093(6)	120
C17–H17A···O7	0.96	2.38	2.785(6)	105
C19–H19A···O9	0.96	1.98	2.433(6)	107
C21–H21A···O8	0.96	1.90	2.398(6)	109

Symmetry codes: (i) 3–*x*, *y*+1/2, –*z*–1/2; (v) 2–*x*, *y*–1/2, –*z*–1/2

Table S4 The dihedral angles for ligand $(HL)^{3-}$ in LOFs **1-3**

LOFs	Two OH groups	SBUs	Dihedral angles (°)	
			Ph/Ph ring	CO_2^{2-}/Ph ring
1	One free; one coordinate	EuO_8	36.6(1)	16.4(1); 1.7(1)
2	One free; one coordinate	GdO_8	37.3(1)	17.0(1); 2.1(1)
3	One free; one coordinate	DyO_8	39.1(1)	17.7(1); 2.6(1)

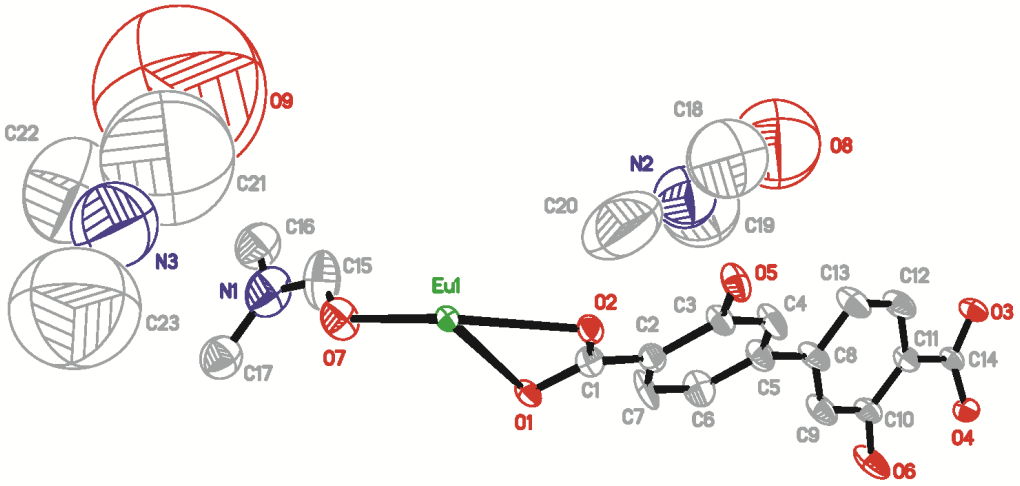

Fig. S1 OPTER drawing (at 50% probability) of the asymmetric unit for LOF **1** (Hydrogen atoms are omitted for clarity).

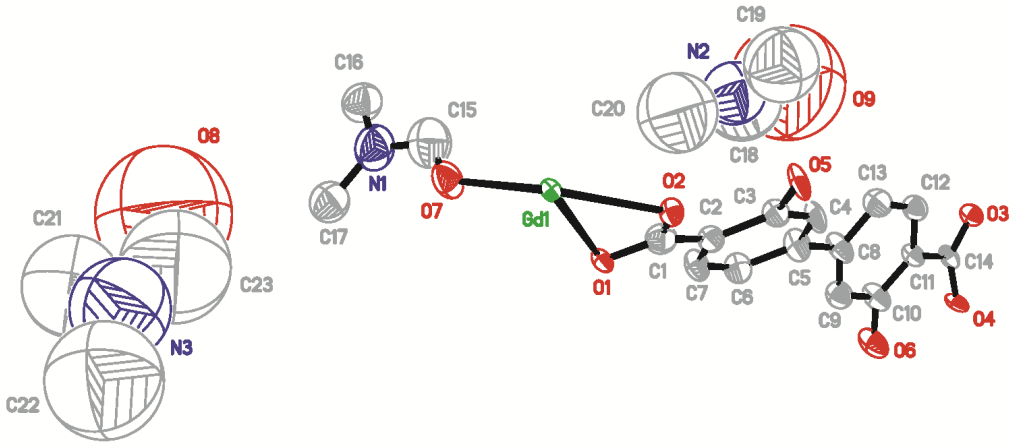

Fig. S2 ORTEP drawing (at 50% probability) of the asymmetric unit for LOF **2** (Hydrogen atoms are omitted for clarity).

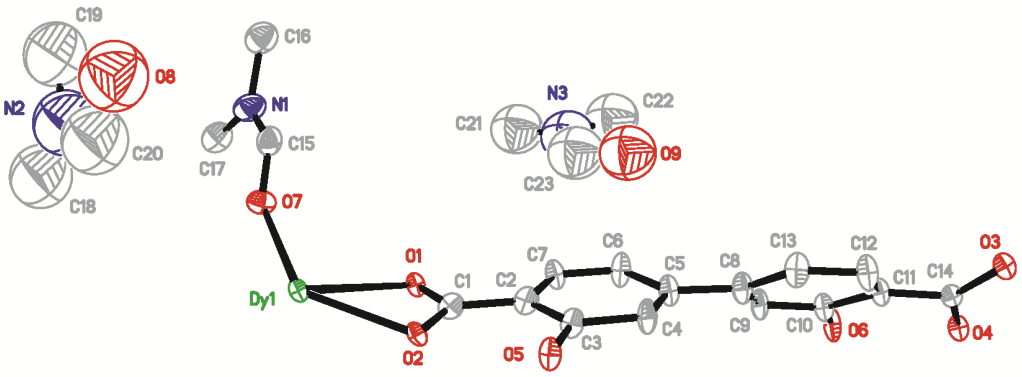

Fig. S3 ORTEP drawing (at 50% probability) of the asymmetric unit for LOF **3** (Hydrogen atoms are omitted for clarity).

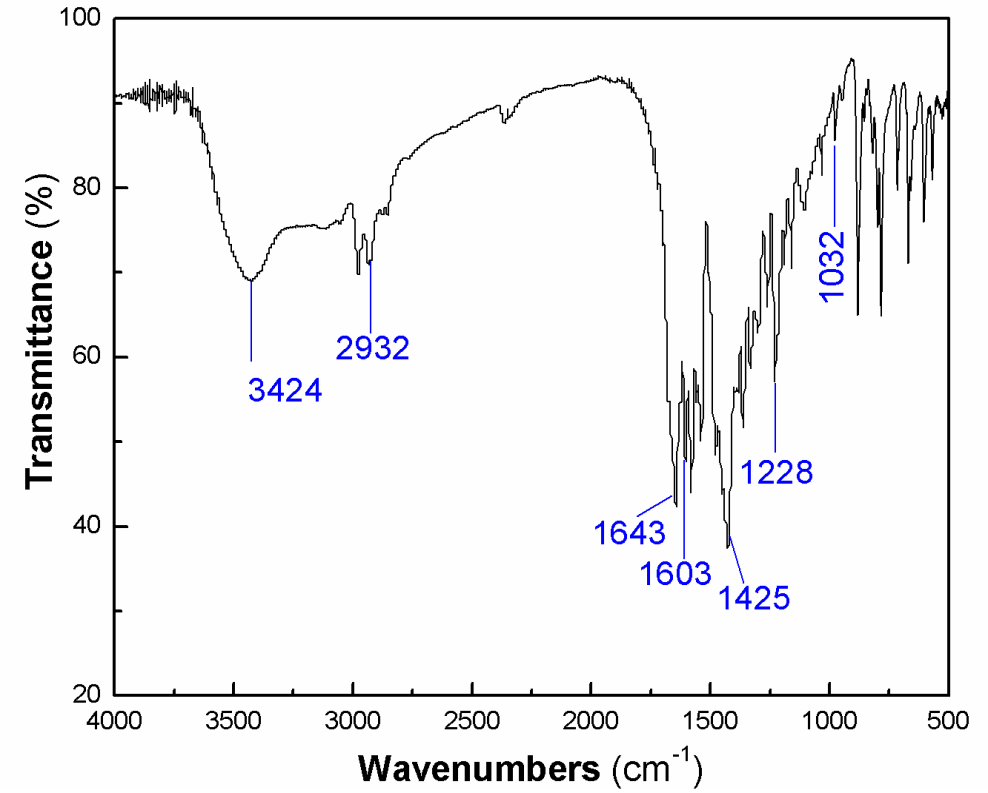

Fig. S4 The IR spectra of LOF **1**.

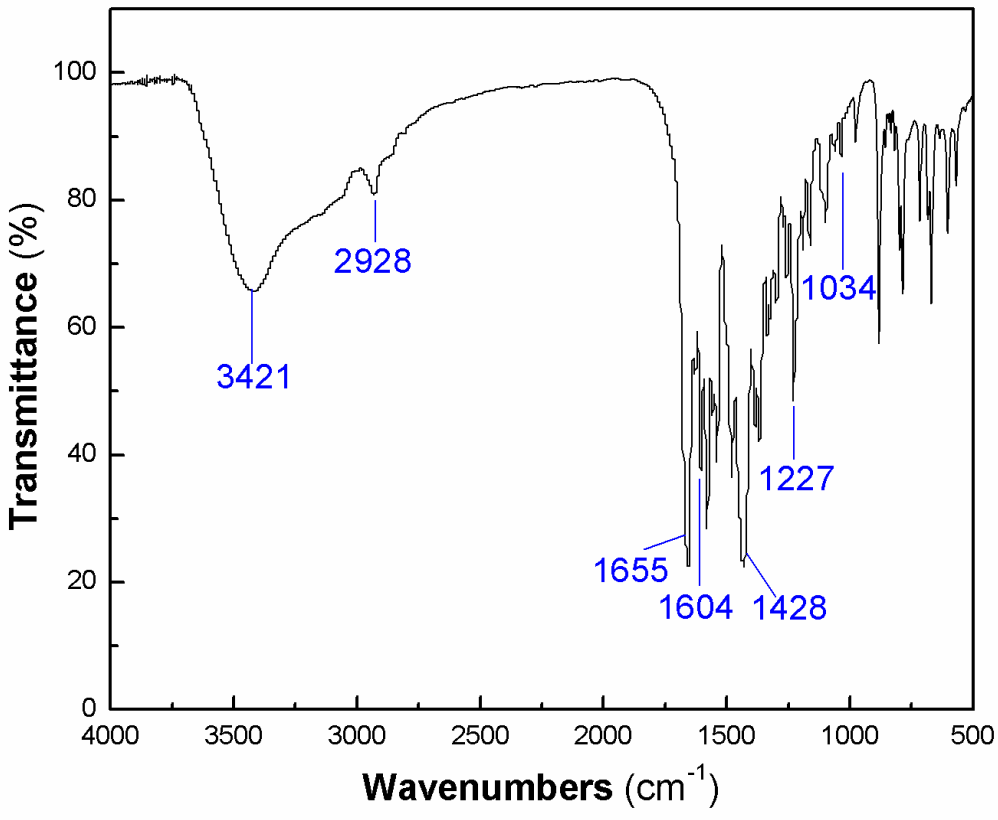

Fig. S5 The IR spectra of LOF **2**.

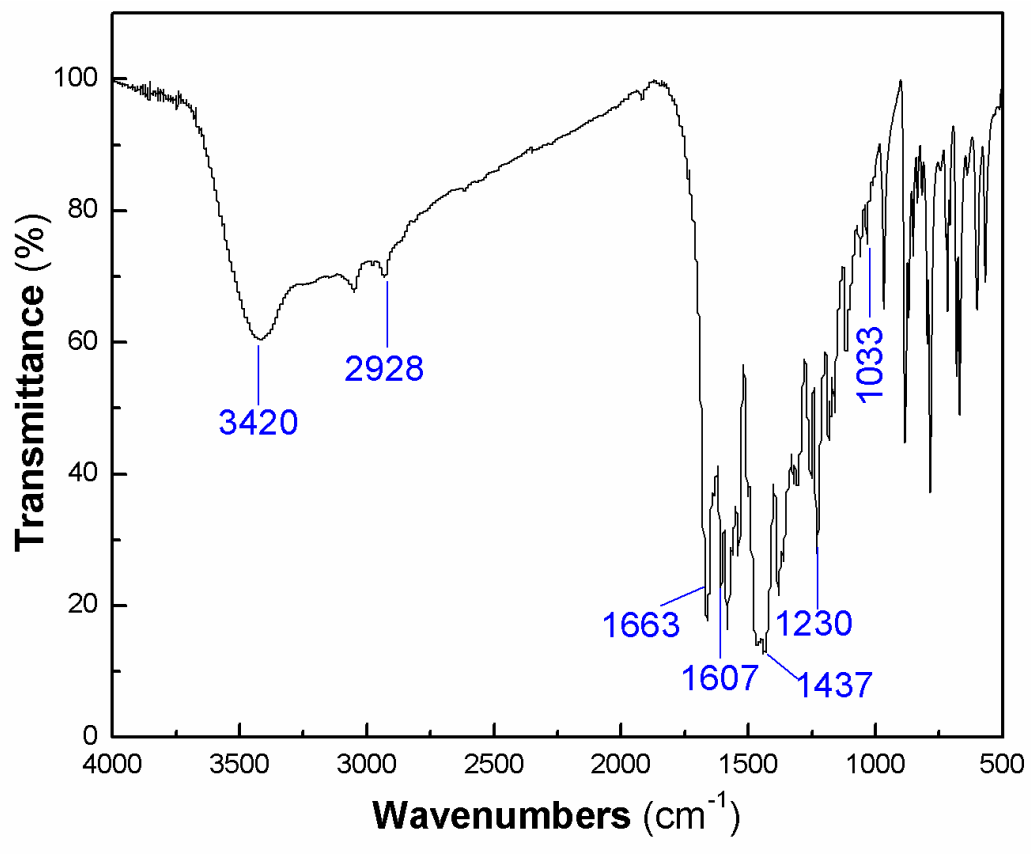

Fig. S6 The IR spectra of LOF **3**.

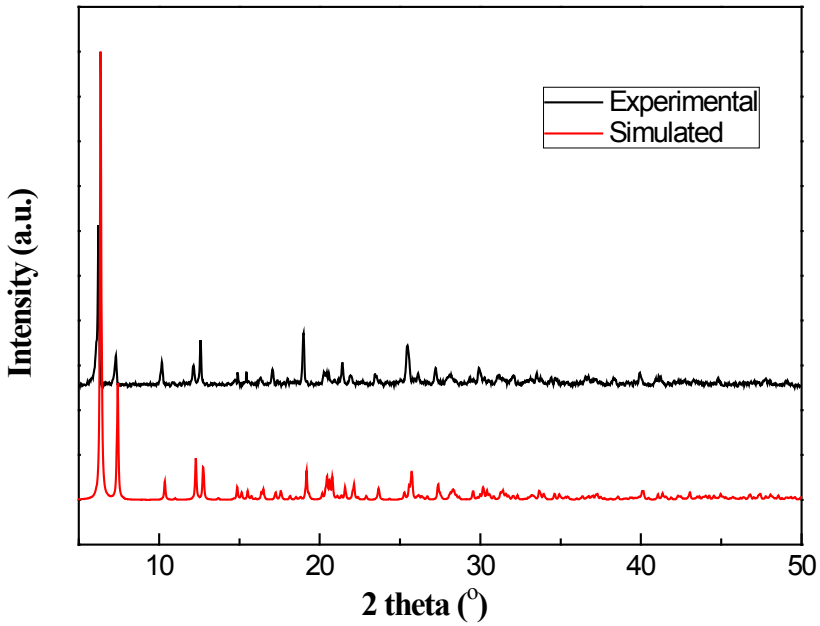

Fig. S7 Experimental and simulated powder X-ray diffraction patterns of LOF **1**.

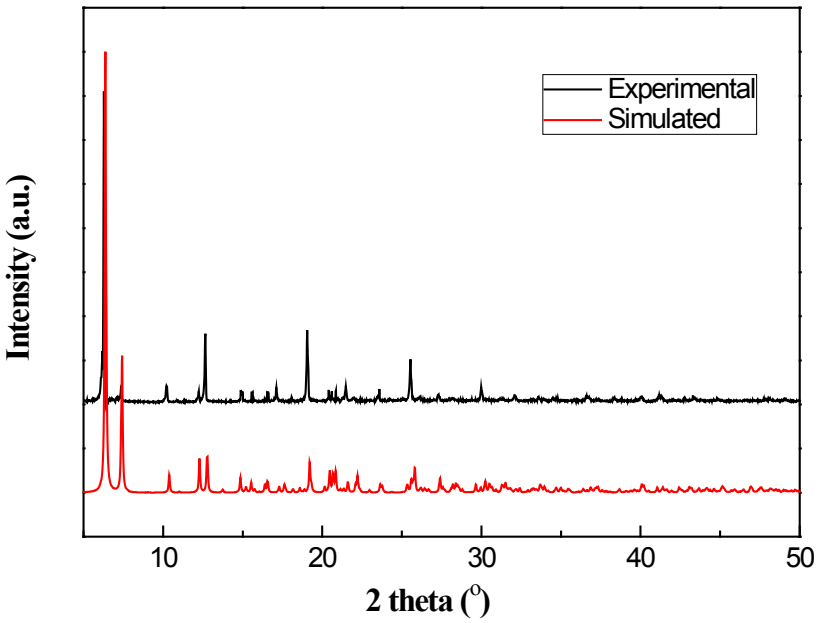

Fig. S8 Experimental and simulated powder X-ray diffraction patterns of LOF **2**.

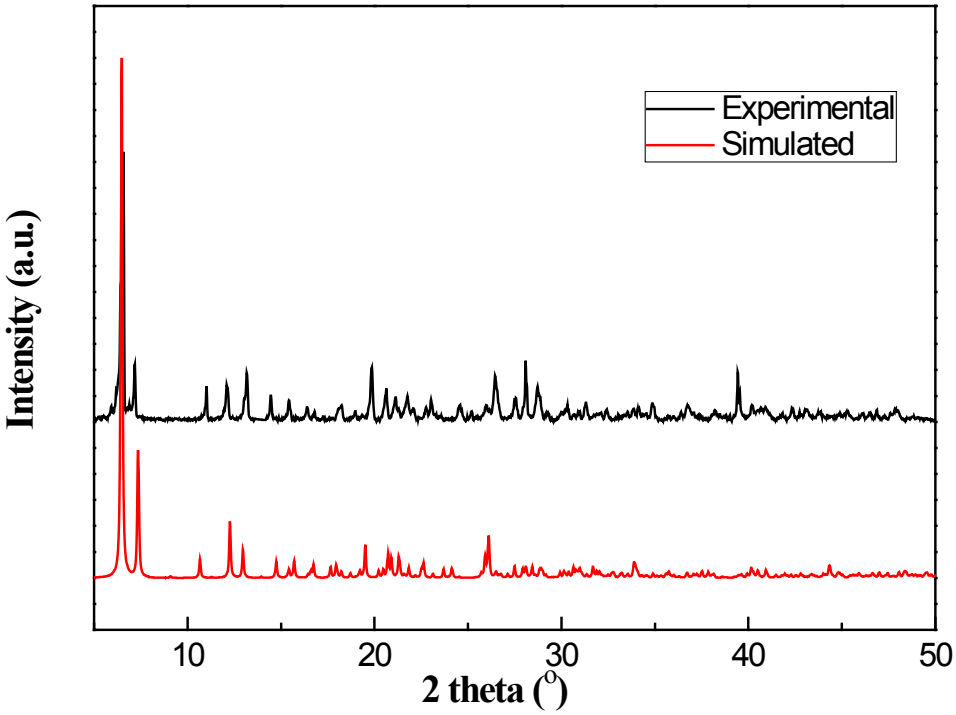

Fig. S9 Experimental and simulated powder X-ray diffraction patterns of LOF **3**.

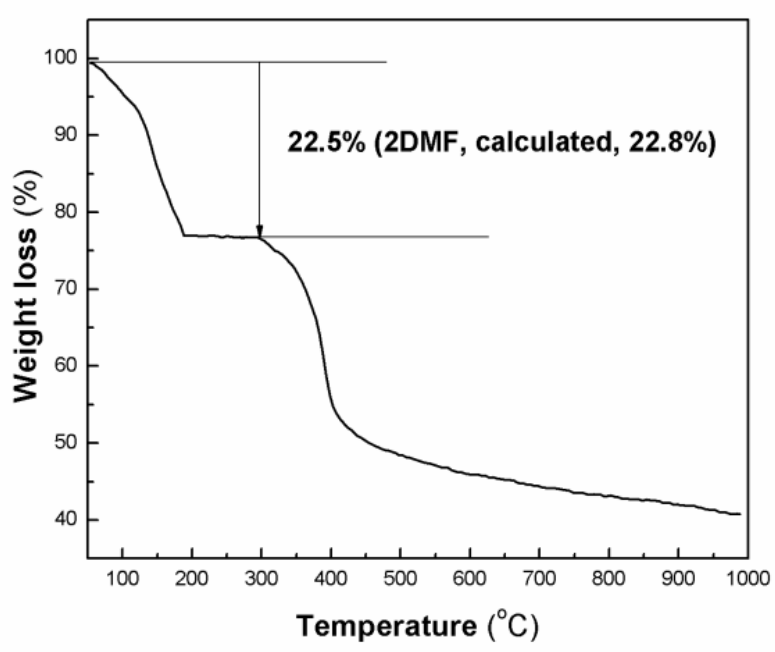

Fig. S10 TGA curve for LOF **1**.

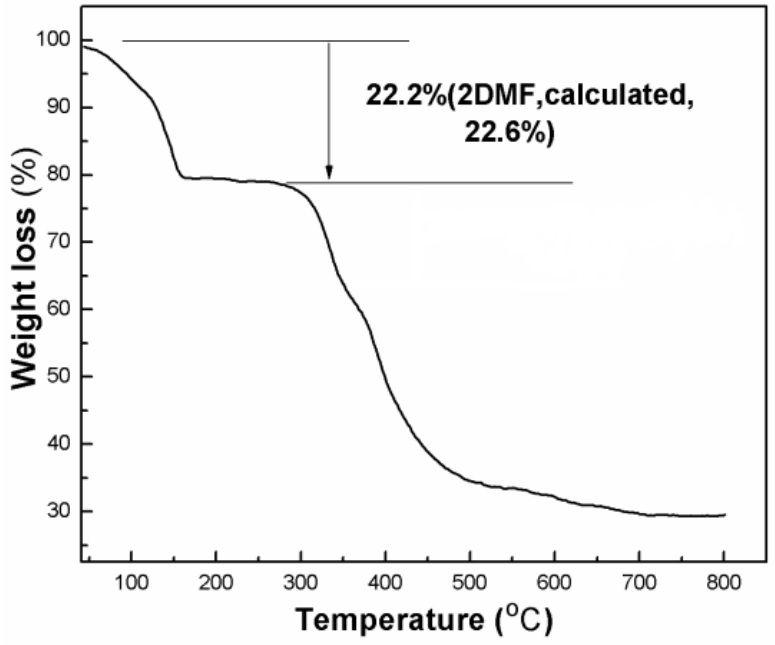

Fig. S11 TGA curve for LOF **2**.

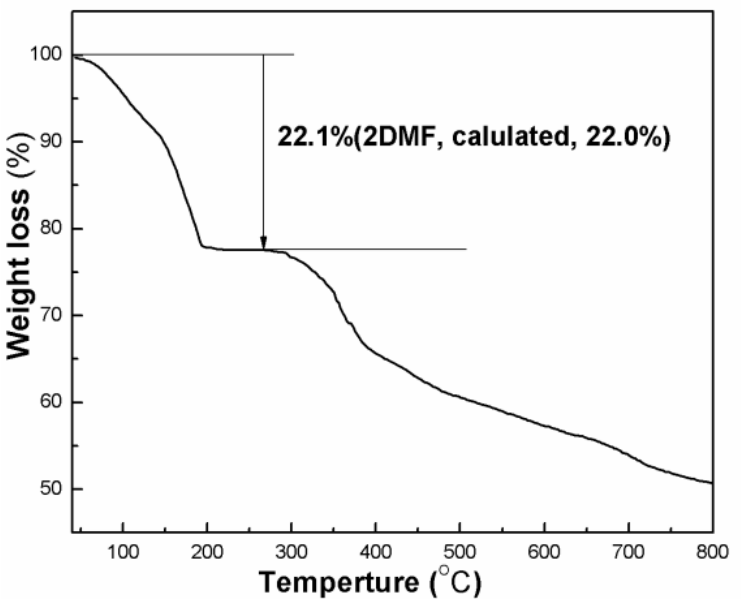

Fig. S12 TGA curve for LOF **3**.

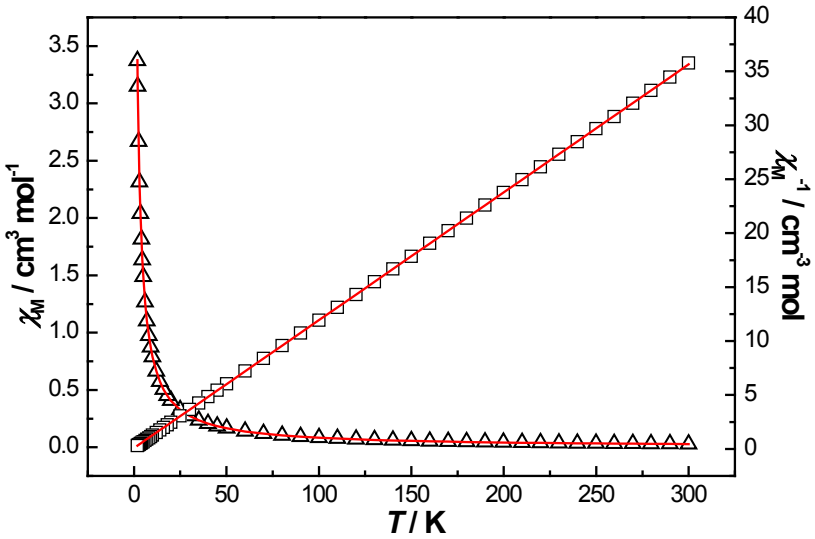

Fig. S13 Variable-temperature susceptibilities for **2** in the form of χ_M and χ_M^{-1} *vs.* *T* under a field of 100 Oe. The solid red lines were derived from the fitting by the Curie-Weiss law.

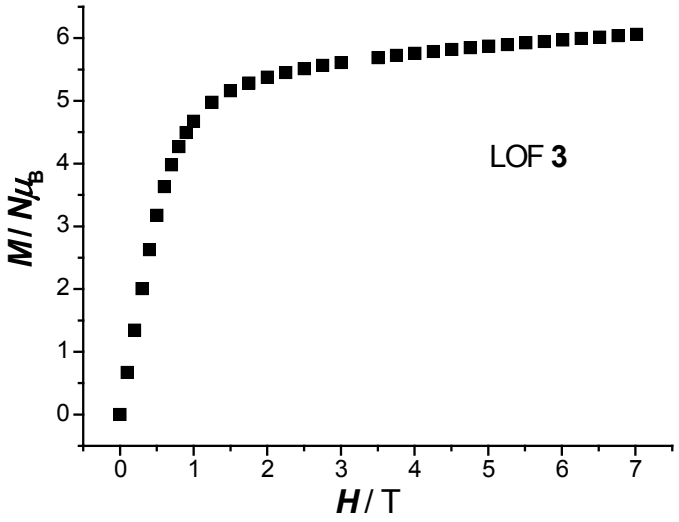

Fig. S14 M-H plot for **3** at 1.8 K.

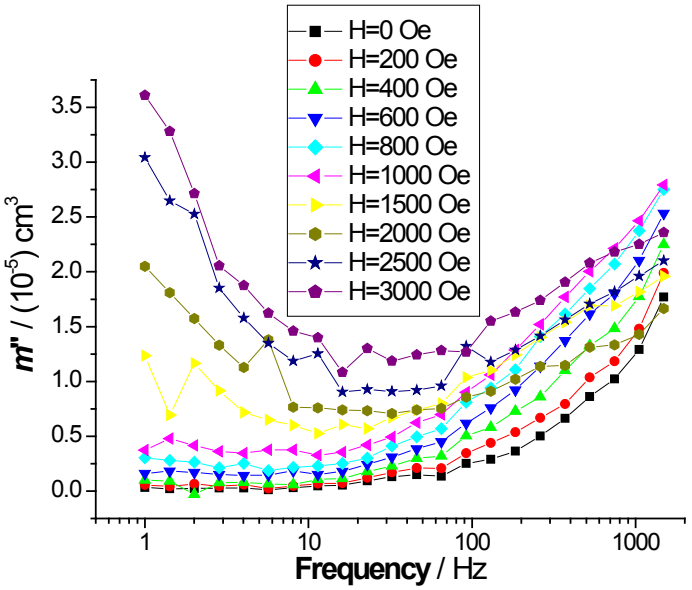

Fig. S15 Frequency dependence of the imaginary χ'' components of the AC susceptibilities measured in different DC applied field for **3** in 1.8 K.