Supplementary Material (ESI) for CrystEngComm

Supporting Information

3D lanthanide-transition-metal−organic frameworks constructed from tetranuclear {Ln_4} SBUs and Cu centers with fsc net

Jing Xu,[a,b] *Weiping Su**[a] *and Maochun Hong*[a]

[a] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China.*

[b] *Graduate School of the Chinese Academy of Sciences, Beijing 100039, P. R. China.*

E-mail: wpsu@fjirsm.ac.cn; Fax: (+86) 591-8377-1575

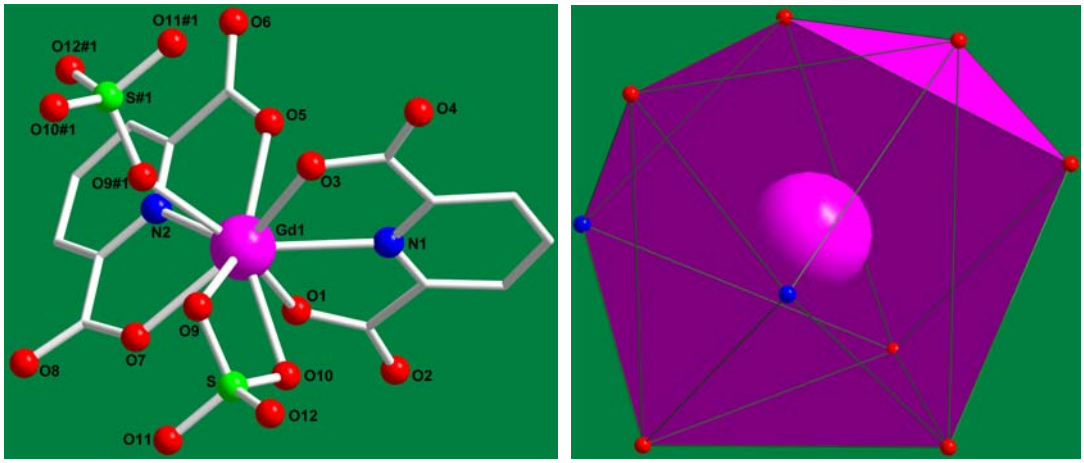

Fig. S1 The coordination environment of the Gd(1) atom in **4**. Symmetry codes for the generated atoms are the same as Table 2.

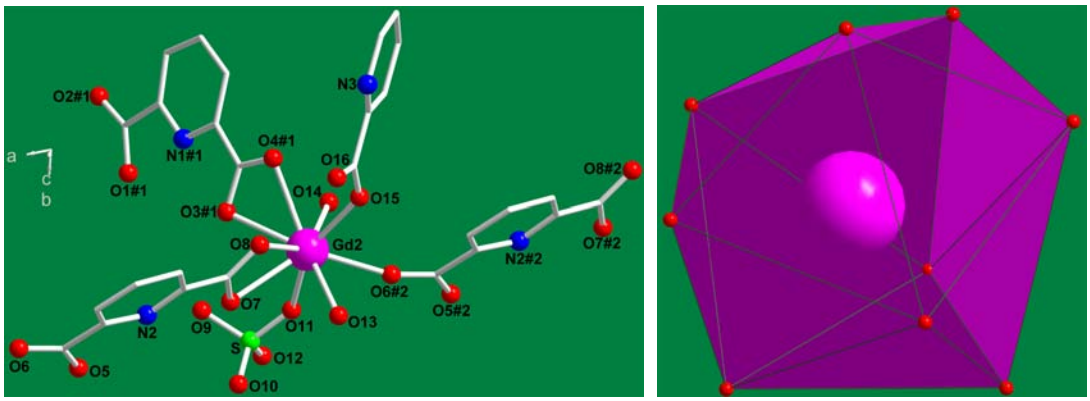

Fig. S2 The coordination environment of the Gd(2) atom in **4**. Symmetry codes for the generated atoms are the same as Table 2.

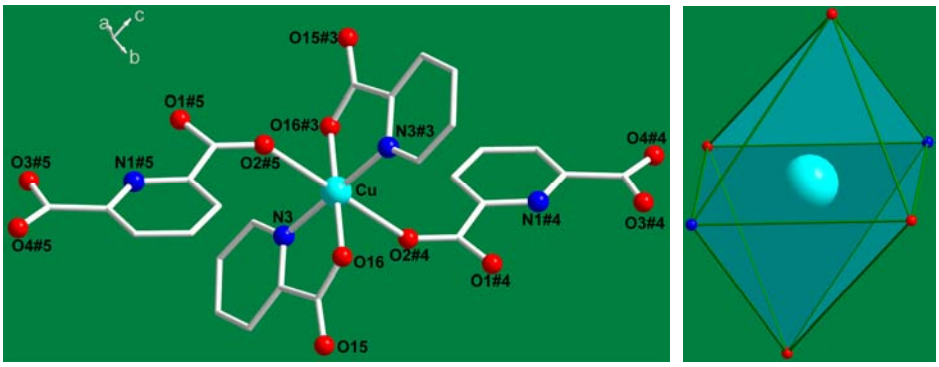

Fig. S3 The coordination environment of the Cu atom in **4**. Symmetry codes for the generated atoms are the same as Table 2.

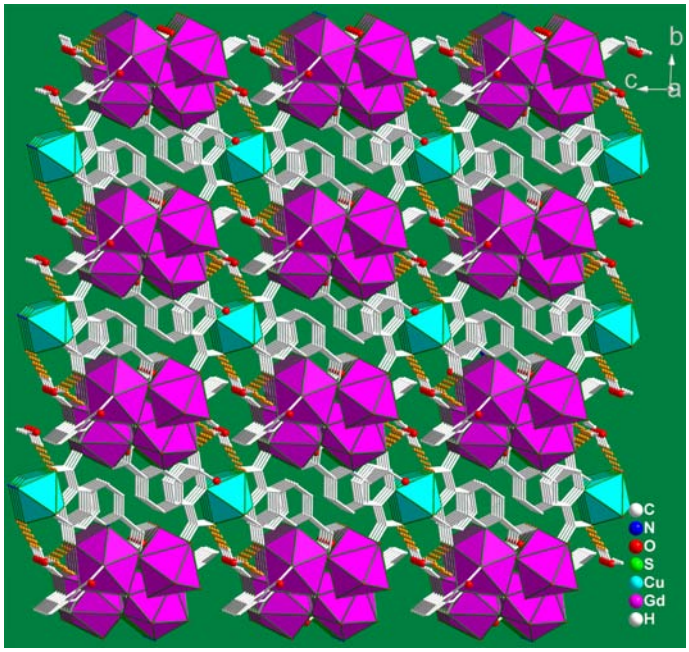

Fig. S4 Hydrogen bonds of the guest water molecules interacting with framework oxygen atoms and coordinated water molecules in the 3D framework of **4** in the *bc* plane. The hydrogen bond interactions are shown as orange dashed lines.

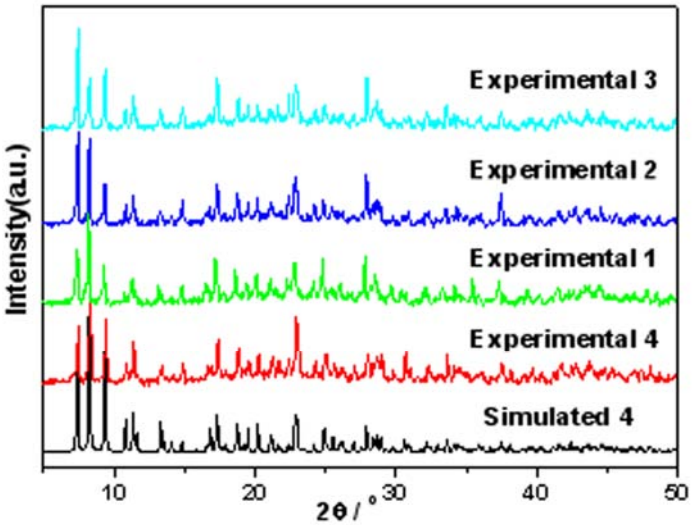

Fig. S5 Simulated PXRD pattern of **4** and experimental PXRD patterns of **1**−**4**.

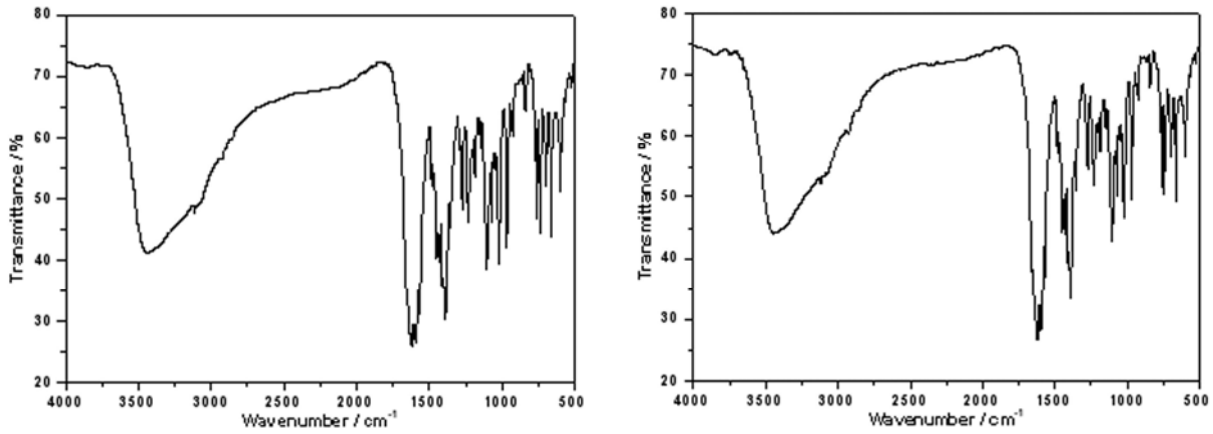

Fig. S6 IR spectra for compounds **1** (left) and **2** (right).

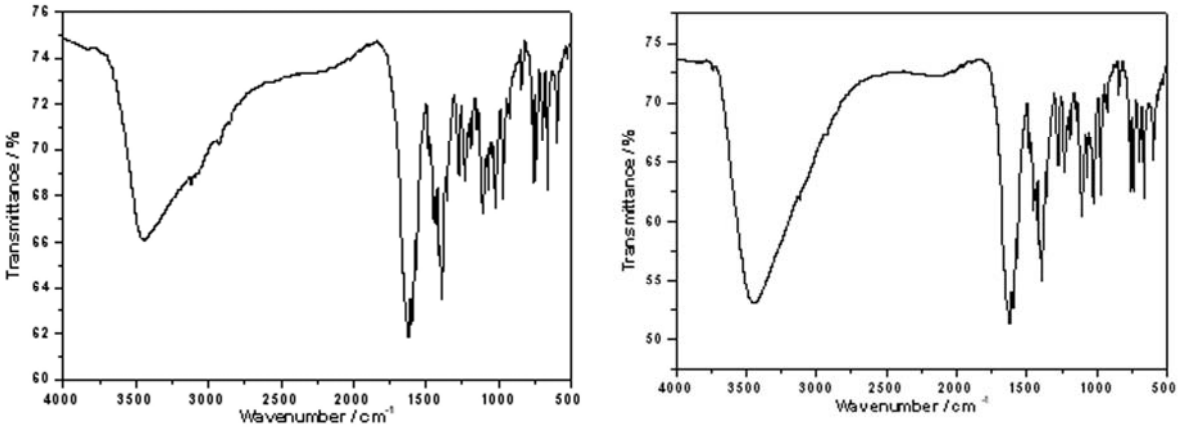

Fig. S7 IR spectra for compounds **3** (left) and **4** (right).

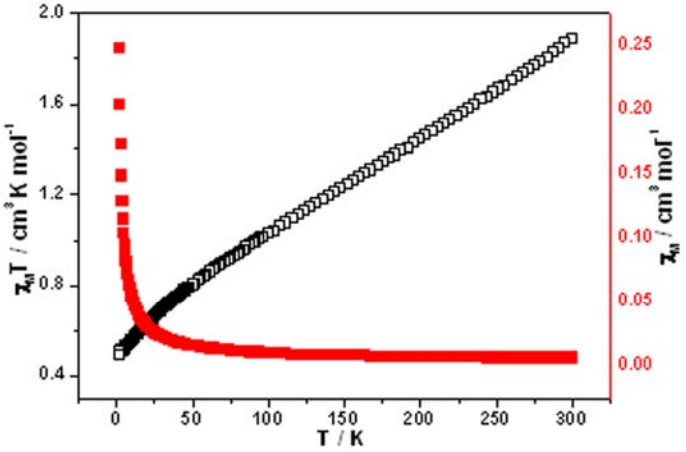

Fig. S8 Temperature dependence of $\chi_M T$ and χ_M for **2** at 1 KOe.

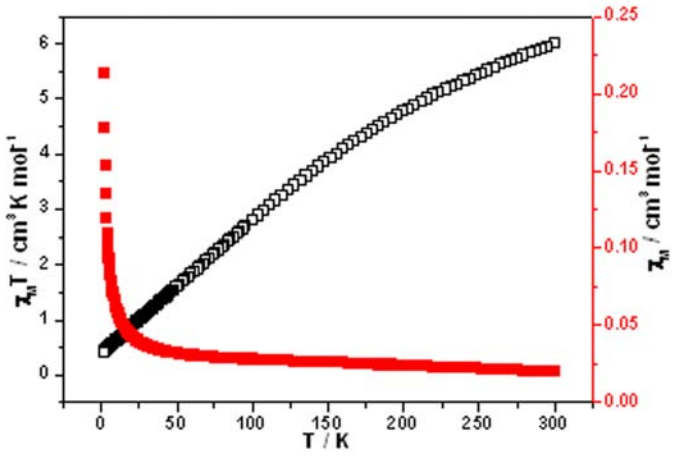

Fig. S9 Temperature dependence of $\chi_M T$ and χ_M for **3** at 1 KOe.

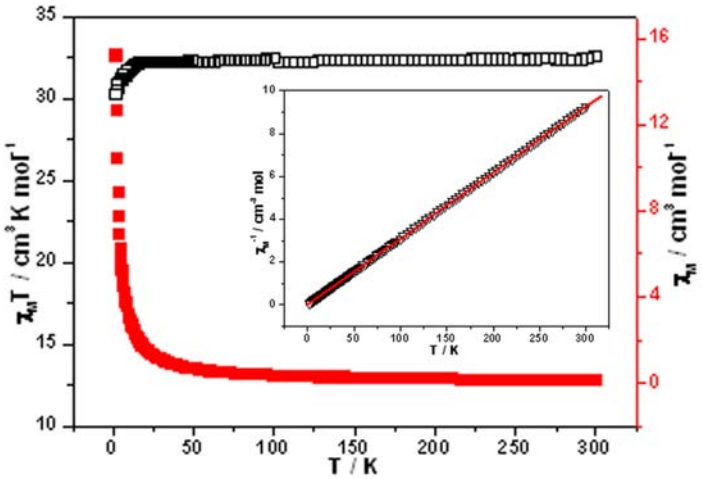

Fig. S10 Temperature dependence of $\chi_M T$, χ_M, and χ_M^{-1}(inset) for **4** at 1 KOe.

Table S1 Hydrogen Bond Lengths (Å) and Bond Angles (°) in **1**−**4**[a]

Compound **1**				
D—H···A	d(D—H)	d(H···A)	d(D···A)	<(DHA)
O(13)—H(13A)···O(6)#2	0.85	2.12	2.751(9)	130.3
O(14)—H(14A)···O(5)#1	0.85	2.18	2.818(8)	131.7
O(14)—H(14B)···O(11)#6	0.85	2.24	3.002(8)	149.1
O(14)—H(14B)···O(12)#6	0.85	2.37	3.090(9)	142.2
O(14)—H(14B)···S#6	0.85	2.81	3.638(6)	166.6
O(17)—H(17B)···O(16)#4	0.85	1.96	2.795(9)	167.0
O(17)—H(17C)···O(1)	0.85	2.00	2.767(9)	148.9
O(17)—H(17C)···O(7)	0.85	2.63	3.150(8)	121.0

[a] Symmetry codes: #1 –*x*+1, -*y*+2, -*z*; #2 *x*-1, *y*, *z*; #4 –*x*, 2-*y*, 1-*z*; #6: -*x*, -*y*+2, -*z*.

Compound **2**				
D—H···A	d(D—H)	d(H···A)	d(D···A)	<(DHA)
O(13)—H(13A)···O(6)#2	0.85	2.03	2.731(12)	139.2
O(14)—H(14A)···O(5)#1	0.85	2.17	2.803(12)	131.2
O(14)—H(14B)···O(11)#6	0.85	2.24	3.006(11)	149.2
O(14)—H(14B)···O(12)#6	0.85	2.38	3.113(12)	144.3
O(14)—H(14B)···S#6	0.85	2.82	3.655(9)	169.1
O(17)—H(17B)···O(16)#4	0.85	1.96	2.800(12)	167.3
O(17)—H(17C)···O(1)	0.85	2.00	2.771(11)	150.4
O(17)—H(17C)···O(7)	0.85	2.64	3.176(11)	122.1

[a] Symmetry codes: #1 –*x*+2, -*y*+1, -*z*; #2 *x*-1, *y*, *z*; #4 –*x*+1, -*y*+1, -*z*+1; #6 –*x*+1, -*y*+1, -*z*.

Compound **3**

D─H···A	d(D─H)	d(H···A)	d(D···A)	<(DHA)
O(13)─H(13A)···O(6)#2	0.85	2.04	2.747(10)	139.9
O(14)─H(14A)···O(5)#1	0.85	2.19	2.795(10)	127.8
O(14)─H(14B)···O(11)#6	0.85	2.25	3.007(9)	148.3
O(14)─H(14B)···O(12)#6	0.85	2.39	3.130(10)	145.9
O(14)─H(14B)···S#6	0.85	2.84	3.678(7)	170.1
O(17)─H(17B)···O(16)#4	0.85	1.96	2.794(11)	167.2
O(17)─H(17C)···O(1)	0.85	2.00	2.771(10)	150.9
O(17)─H(17C)···O(7)	0.85	2.64	3.181(10)	122.6

[a] Symmetry codes: #1 –*x*+2, -*y*+1, -*z*; #2 *x*-1, *y*, *z*; #4 –*x*+1, -*y*+1, -*z*+1; #6 –*x*+1, -*y*+1, -*z*.

Compound **4**

D─H···A	d(D─H)	d(H···A)	d(D···A)	<(DHA)
O(13)─H(13A)···O(6)#2	0.85	1.87	2.707(9)	168.9
O(14)─H(14A)···O(5)#6	0.85	2.16	2.786(9)	130.7
O(14)─H(14B)···O(11)#7	0.85	2.26	2.995(9)	144.7
O(14)─H(14B)···O(12)#7	0.85	2.35	3.114(10)	150.1
O(14)─H(14B)···S#7	0.85	2.81	3.655(7)	171.0
O(17)─H(17B)···O(16)#4	0.85	1.95	2.788(10)	167.4
O(17)─H(17C)···O(1)	0.85	1.97	2.751(10)	151.4
O(17)─H(17C)···O(7)	0.85	2.64	3.163(9)	120.6

[a] Symmetry codes: #2 x-1, y, z; #4 1-*x*, 2-*y*, 1-*z*; #6 –*x*+2, -*y*+2, -*z*; #7 –*x*+1, -*y*+2, -*z*.