Supporting Information

Three Pillared-Layer 3d-4f Heterometallic Frameworks Based on Tetranuclear Lanthanide Clusters

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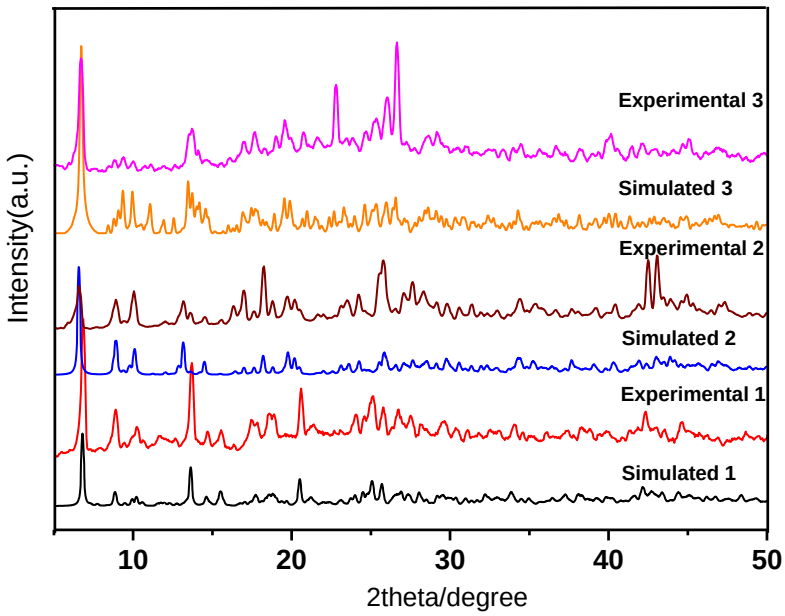

Figure S1. The experimental and simulated PXRD patterns of compounds **1**-**3**.

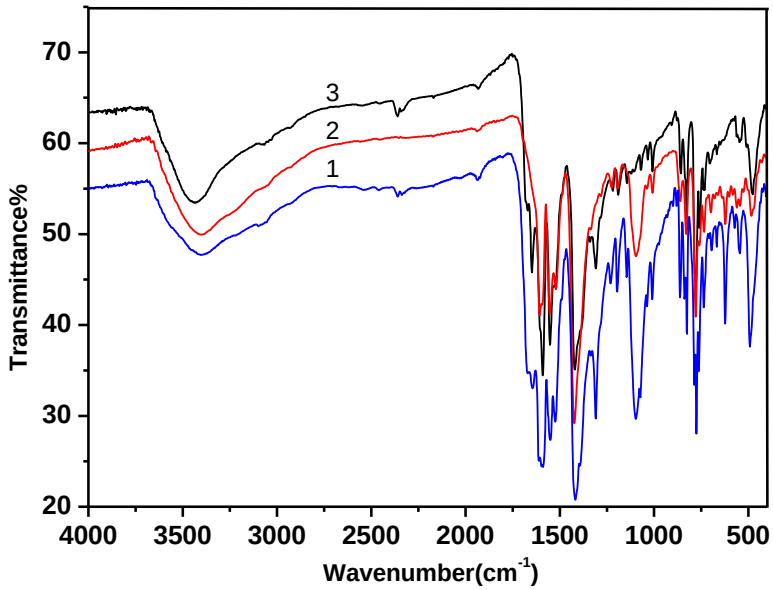

Figure S2. The IR spectra of compounds **1**-**3**.

Table S1. Selected Bond Lengths (Å) for Compounds **1-3**

Compound 1			
Gd(1)-O(1)	2.423(8)	Cu(2)-N(8)	1.904(1)
Gd(1)-O(1W)	2.390(9)	Cu(2)-N(9)B	1.905(1)
Gd(1)-O(2)	2.465(9)	Cu(3)-N(3)C	2.045(9)
Gd(1)-O(3)	2.511(7)	Cu(3)-I(1)	2.610(2)
Gd(1)-O(4)	2.390(9)	Cu(3)-I(2)	2.611(2)
Gd(1)-O(5)	2.328(9)	Cu(3)-I(7)D	2.874(2)
Gd(1)-O(7)	2.349(8)	Cu(4)-N(2)	2.038(1)
Gd(1)-O(11)	2.285(8)	Cu(4)-I(1)	2.652(2)
Gd(2)-O(2W)	2.378(1)	Cu(4)-I(2)	2.618(2)
Gd(2)-O(3W)	2.438(1)	Cu(4)-I(3)	2.841(2)
Gd(2)-O(4W)	2.378(1)	Cu(5)-N(1)C	2.051(1)
Gd(2)-O(6)	2.335(8)	Cu(5)-I(2)	2.894(2)
Gd(2)-O(8)	2.356(1)	Cu(5)-I(3)	2.624(2)
Gd(2)-O(9)	2.331(8)	Cu(5)-I(4)	2.574(9)
Gd(2)-O(15)	2.450(9)	Cu(6)-N(6)	2.006(1)
Gd(2)-O(16)	2.601(1)	Cu(6)-I(3)	2.665(2)
Gd(3)-O(5W)	2.646(1)	Cu(6)-I(4)	2.653(1)
Gd(3)-O(6W)	2.422(1)	Cu(6)-I(5)	2.813(3)
Gd(3)-O(10)	2.263(8)	Cu(7)-N(7)E	2.023(1)
Gd(3)-O(14)	2.361(1)	Cu(7)-I(3)	2.844(3)
Gd(3)-O(17)	2.330(9)	Cu(7)-I(5)	2.652(2)
Gd(3)-O(19)	2.422(9)	Cu(7)-I(6)	2.631(2)
Gd(3)-O(20)	2.550(9)	Cu(8)-N(10)	2.045(1)
Gd(3)-O(23)	2.322(8)	Cu(8)-I(5)	2.612(2)
Gd(4)-O(7W)	2.395(9)	Cu(8)-I(6)	2.613(2)
Gd(4)-O(8W)	2.412(1)	Cu(8)-I(7)	2.902(3)
Gd(4)-O(9W)	2.436(1)	Cu(9)-N(5)E	2.001(1)
Gd(4)-O(10W)	2.334(1)	Cu(9)-I(5)	2.991(3)
Gd(4)-O(18)	2.247(1)	Cu(9)-I(7)	2.678(3)
Gd(4)-O(21)	2.431(1)	Cu(9)-I(8)	2.584(2)
Gd(4)-O(22)	2.566(1)	Cu(10)-N(12)	2.060(1)
Gd(4)-O(24)	2.308(9)	Cu(10)-I(2)F	2.880(3)
Cu(1)-N(11)A	1.890(1)	Cu(10)-I(7)	2.628(2)
Cu(1)-N(4)	1.942(1)	Cu(10)-I(8)	2.620(2)

Symmetry transformations used to generate equivalent atoms: A: *x*-1, *y*-1, *z*; B: *x*-1, *y*, *z*; C: *x*-1, -*y*, *z*-1/2; D: *x*, *y*-1, *z*; E: *x*-1, -*y*+1, *z*-1/2; F: *x*, *y*+1, *z*.

Compound 2

La(1)-O(1)	2.472(6)	La(2)-O(12)C	2.475(5)
La(1)-O(2)A	2.564(6)	Cu(1)-N(1)	2.004(7)
La(1)-O(3)	2.481(5)	Cu(1)-I(1)	2.605(1)
La(1)-O(5)	2.443(5)	Cu(1)-I(2)	2.666(1)
La(1)-O(8)	2.431(5)	Cu(1)-I(3)	2.953(2)
La(1)-O(9)	2.449(5)	Cu(2)-N(2)D	2.013(7)
La(1)-O(11)B	2.702(5)	Cu(2)-I(1)	2.650(1)
La(2)-O(1W)	2.578(6)	Cu(2)-I(1)E	2.703(1)
La(2)-O(2W)	2.564(7)	Cu(2)-I(2)	2.733(1)
La(2)-O(4)	2.469(5)	Cu(3)-N(3)	2.015(1)
La(2)-O(6)	2.554(5)	Cu(3)-I(2)F	2.635(1)
La(2)-O(7)B	2.467(5)	Cu(3)-I(3)	2.613(1)
La(2)-O(10)B	2.513(5)	Cu(4)-N(4)F	1.883(7)
La(2)-O(11)C	2.668(5)	Cu(4)-N(4)	1.883(7)

Symmetry transformations used to generate equivalent atoms: A: -*x*+1/2, -*y*+3/2, -*z*+1; B: -*x*+1/2, *y*+1/2, -*z*+1/2; C: *x*, *y*+1, *z*; D: *x*-1/2, *y*+1/2, *z*; E: -*x*, -*y*+2, -*z*+1; F: -*x*, *y*, -*z*+1/2.

Compound 3

La(1)-O(6)	2.593(8)	La(4)-O(28)D	2.624(7)
La(1)-O(7)	2.501(9)	Na-O(3W)	2.328(13)
La(1)-O(14)	2.608(8)	Na-O(6)	2.461(10)
La(1)-O(17)	2.735(8)	Na-O(9)D	2.930(12)
La(1)-O(19)	2.441(8)	Na-O(10)D	2.412(11)
La(1)-O(1W)	2.762(1)	Na-O(19)	2.841(10)
La(1)-O(22)	2.578(8)	Na-O(20)D	2.497(9)
La(1)-O(27)	2.612(8)	Na-O(27)	2.423(9)
La(1)-O(28)A	2.641(8)	Cu(1)-I(1)	2.579(3)
La(2)-O(1)	2.393(8)	Cu(1)-I(1)E	2.571(2)
La(2)-O(2W)	2.522(1)	Cu(1)-N(1)	1.992(1)
La(2)-O(4)	2.476(9)	Cu(2)-I(2)	2.567(3)
La(2)-O(5)	2.469(9)	Cu(2)-I(3)	2.586(3)
La(2)-O(16)	2.475(9)	Cu(2)-N(8)F	1.970(1)
La(2)-O(17)	2.647(7)	Cu(3)-I(2)	2.700(2)
La(2)-O(21)	2.466(9)	Cu(3)-I(3)	2.713(2)
La(2)-O(22)	2.722(8)	Cu(3)-I(4)	2.695(2)
La(3)-O(3)	2.527(8)	Cu(3)-N(2)	2.023(1)
La(3)-O(11)	2.457(1)	Cu(4)-I(3)	2.750(2)
La(3)-O(15)	2.446(1)	Cu(4)-N(3)B	1.942(1)
La(3)-O(18)	2.666(7)	Cu(4)-N(6)F	1.930(1)
La(3)-O(23)B	2.496(9)	Cu(5)-I(2)	2.766(2)
La(3)-O(24)B	2.698(8)	Cu(5)-I(4)	2.644(2)
La(3)-O(25)	2.535(9)	Cu(5)-I(5)	2.695(3)
La(3)-O(26)C	2.532(9)	Cu(5)-N(7)F	2.048(1)
La(4)-O(8)B	2.486(8)	Cu(6)-I(4)	2.748(2)

La(4)-O(9)	2.457(9)	Cu(6)-I(5)	2.672(3)
La(4)-O(12)	2.463(1)	Cu(6)-I(6)	2.671(2)
La(4)-O(13)B	2.482(8)	Cu(6)-N(4)B	2.036(1)
La(4)-O(18)	2.659(8)	Cu(7)-I(5)	2.566(2)
La(4)-O(20)	2.454(8)	Cu(7)-I(6)	2.514(2)
La(4)-O(24)B	2.535(8)	Cu(7)-N(5)G	1.971(11)

Symmetry transformations used to generate equivalent atoms: A: -*x*+2, -*y*, -*z*+1; B: *x*-1, *y*, *z*; C: -*x*+1, -*y*+1, -*z*+1; D: -*x*+1, -*y*, -*z*+1; E: -*x*+4, -*y*+1, -*z*+2; F: *x*, *y*, *z*+1; G: *x*+1, *y*, *z*+1.

Table S2. Hydrogen Bond Lengths (Å) and Bond Angles (°) for compounds **1**[a]

D-H···A	d(D-H)	d(H···A)	d(D···A)	<DHA
O2W-H(2WB)···O8W^{G}	0.93	2.38	3.25(1)	158.9
O3W-H(3WB)···O12^{G}	0.88	2.05	2.76(1)	137.5
O4W-H(4WA)···O11	0.88	2.28	2.89(1)	127.1
O4W-H(4WB)···O5	0.89	2.48	3.10(1)	128.6
O5W-H(5WB)···O12	0.94	2.11	2.95(1)	149.4
O6W-H(6WB)···O16	0.86	2.08	2.79(1)	140.5
O7W-H(7WA)···O14	0.85	2.48	3.09(1)	129.6
O7W-H(7WB)···O1^{F}	0.85	2.27	2.69(1)	111.4
O8W-H(8WB)···O2^{H}	0.86	2.38	3.18(2)	155.7
O9W-H(9WA)···O14^{I}	0.87	2.04	2.87(2)	159.5
O9W-H(9WB)···O13W^{F}	0.87	2.44	3.30(3)	169.2
O11W-H(11A)···O4^{F}	0.85	2.28	2.86(2)	125.5
O12W-H(12A)···O3W	0.85	2.09	2.74(2)	132.6
O13W-H(13A)···O21^{D}	0.85	2	2.82(3)	161.9
O13W-H(13B)···O12W^{H}	0.85	2.37	2.90(3)	121.1

[a] Symmetry codes: D: *x*, *y*-1, *z*; F: *x*, *y*+1, *z*.; G: *x*, -*y*+1, *z*+1/2; H: *x*, -*y*+1, *z*-1/2; I: *x*, -*y*+2, *z*-1/2.