Electronic Supplementary Material (ESI) for Dalton Transactions

A Family of Three-Dimensional 3d-4f and 4d-4f Heterometallic Coordination Polymers Based on Mixed Isonicotinate and 2-Sulfobenzoate Ligands: Syntheses, Structures and Photoluminescent Properties

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Figure S1-S17. As-synthesized and calculated powder X-ray diffraction (XRD) patterns of **1-17**.

Figure S18-S20. Thermogravimetric analysis (TGA) curves of **1-17**.

Table S1. Selected bond lengths [Å] for **1-17**.

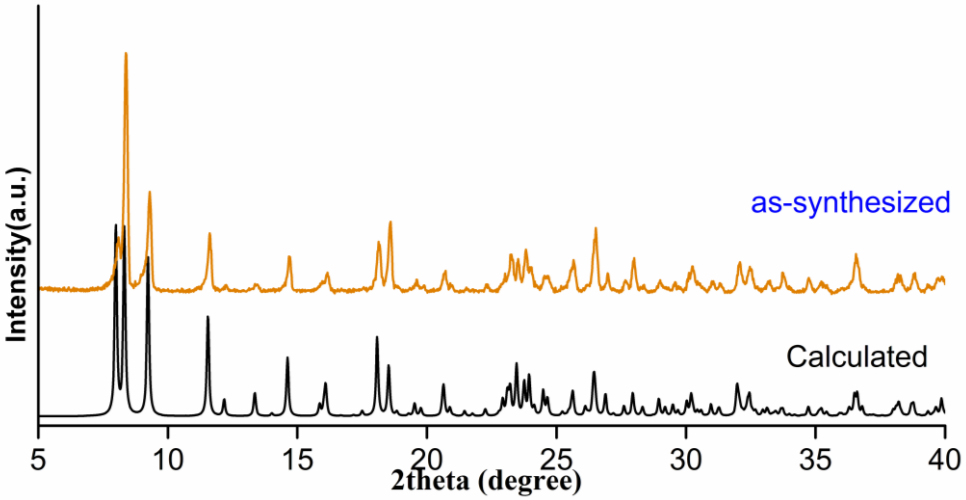

Figure S1. As-synthesized and calculated powder XRD patterns of **1**.

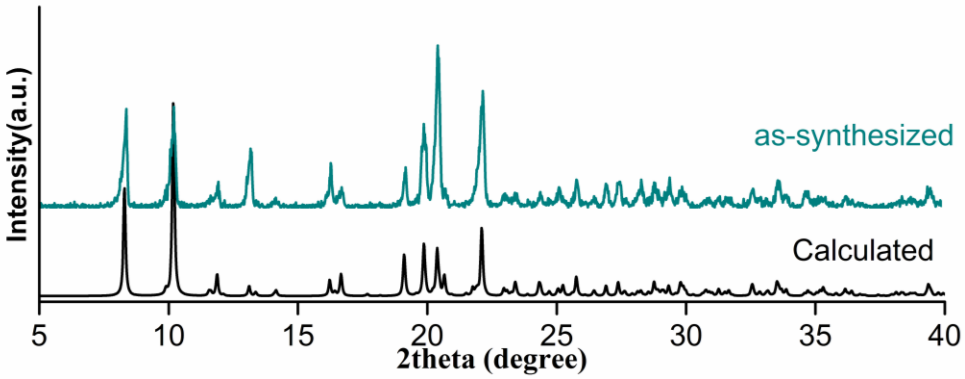

Figure S2. As-synthesized and calculated powder XRD patterns of **2**.

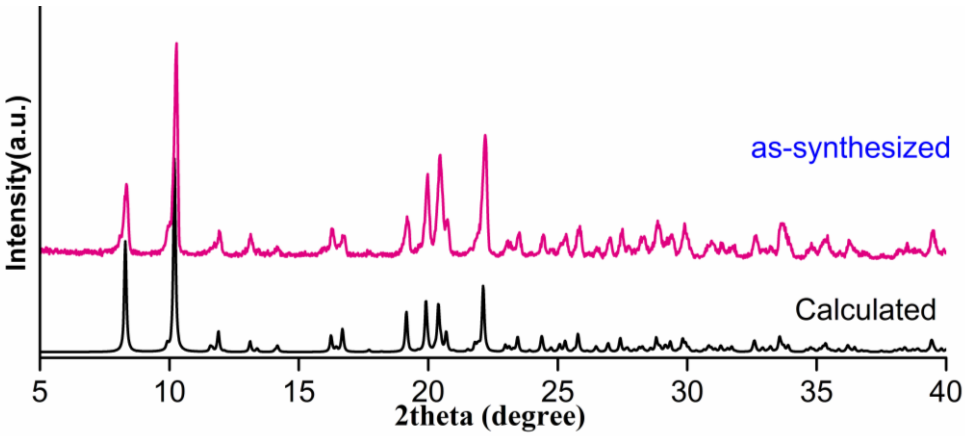

Figure S3. As-synthesized and calculated powder XRD patterns of **3**.

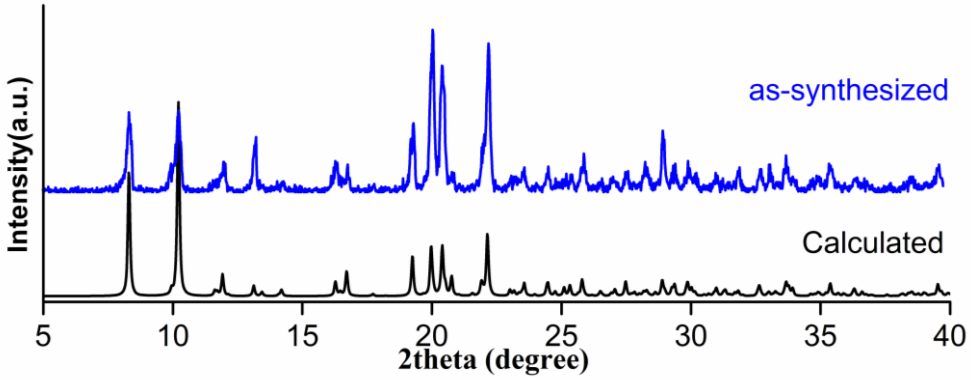

Figure S4. As-synthesized and calculated powder XRD patterns of **4**.

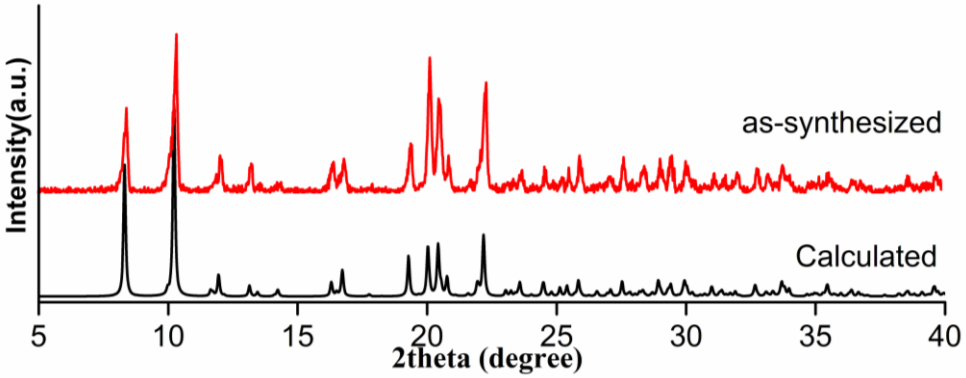

Figure S5. As-synthesized and calculated powder XRD patterns of **5**.

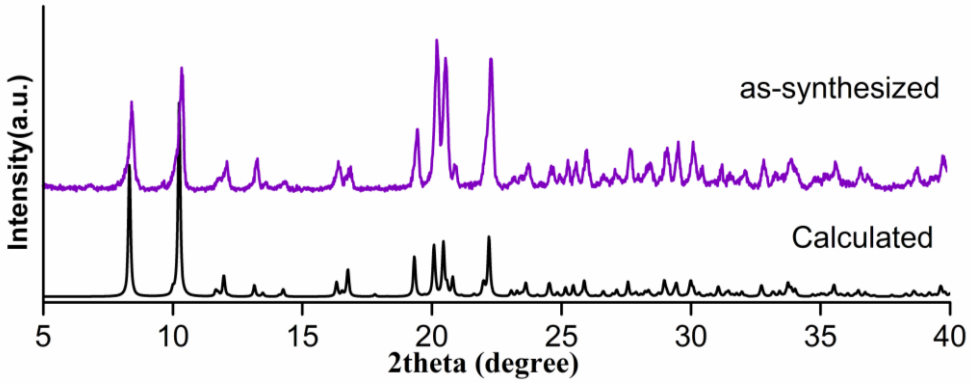

Figure S6. As-synthesized and calculated powder XRD patterns of **6**.

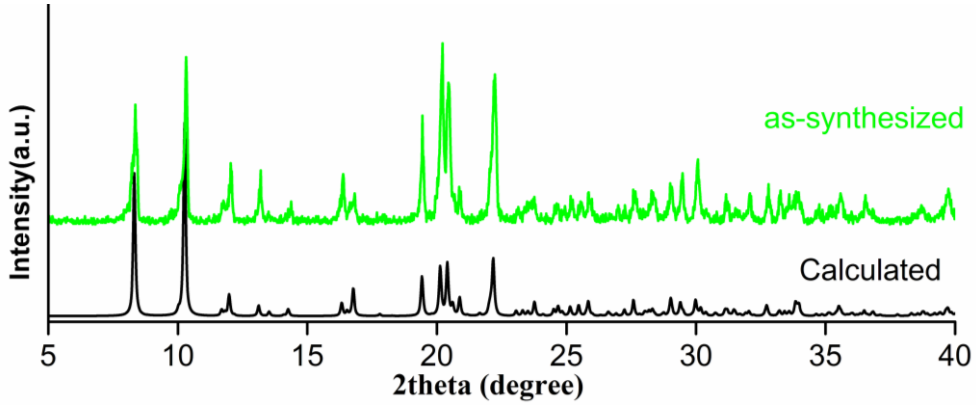

Figure S7. As-synthesized and calculated PXRD powder XRD patterns of **7**.

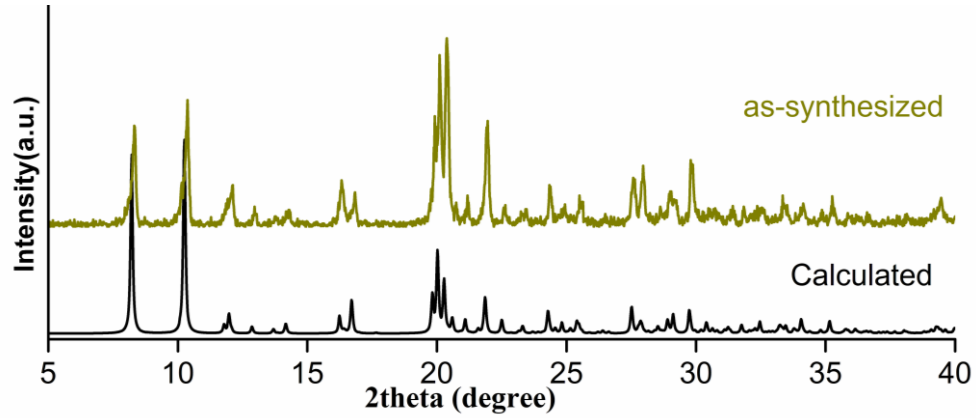

Figure S8. As-synthesized and calculated powder XRD patterns of **8**.

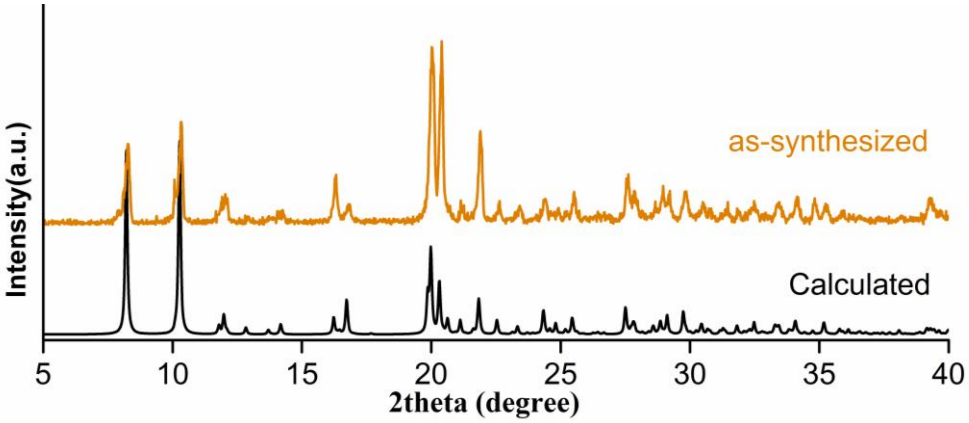

Figure S9. As-synthesized and calculated powder XRD patterns of **9**.

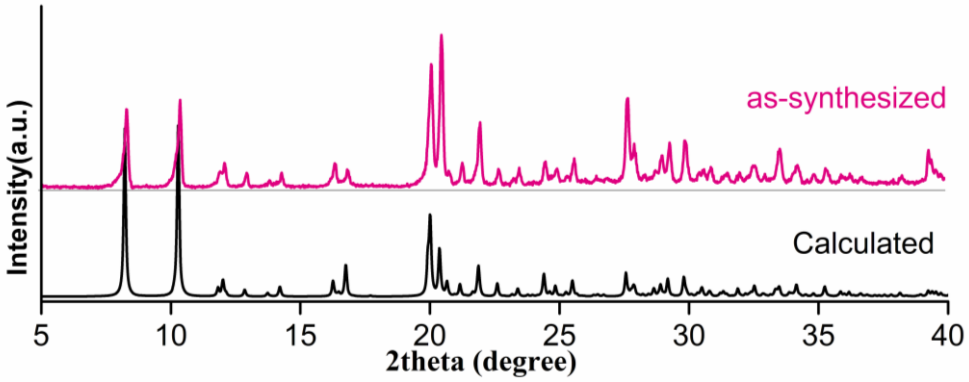

Figure S10. As-synthesized and calculated powder XRD patterns of **10**.

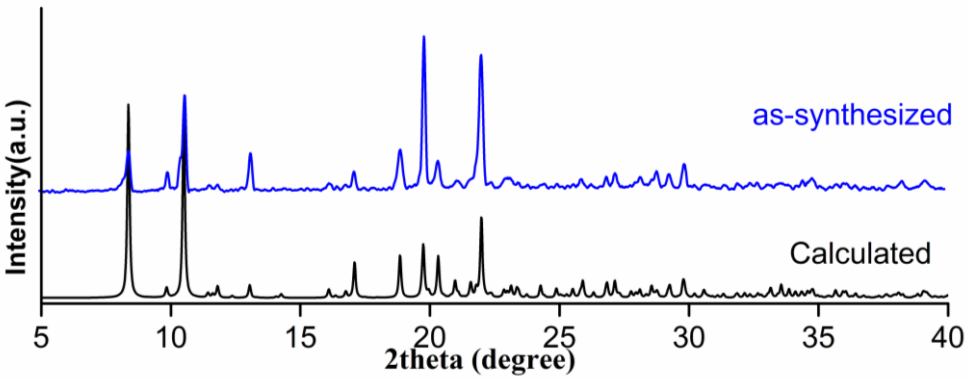

Figure S11. As-synthesized and calculated powder XRD patterns of **11**.

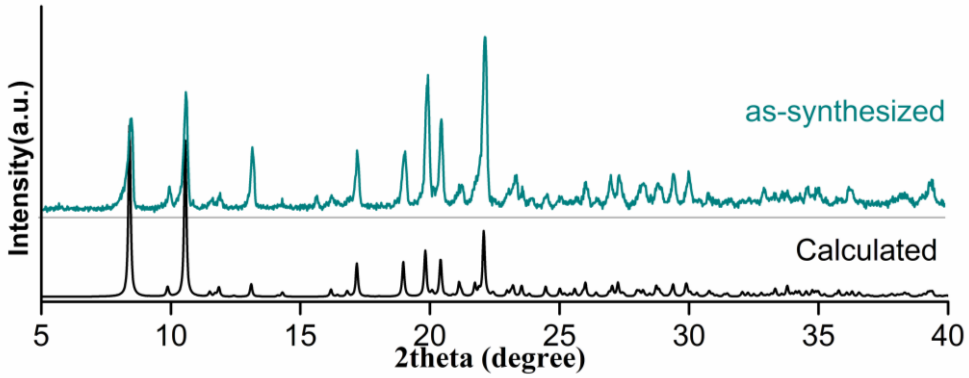

Figure S12. As-synthesized and calculated powder XRD patterns of **12**.

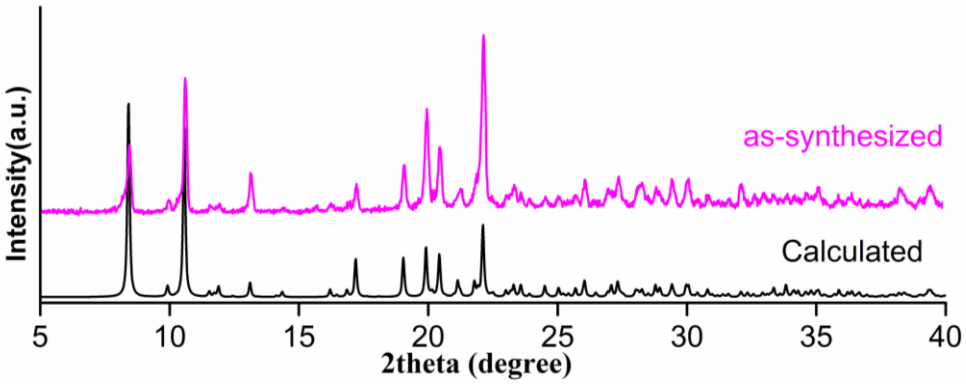

Figure S13. As-synthesized and calculated powder XRD patterns of **13**.

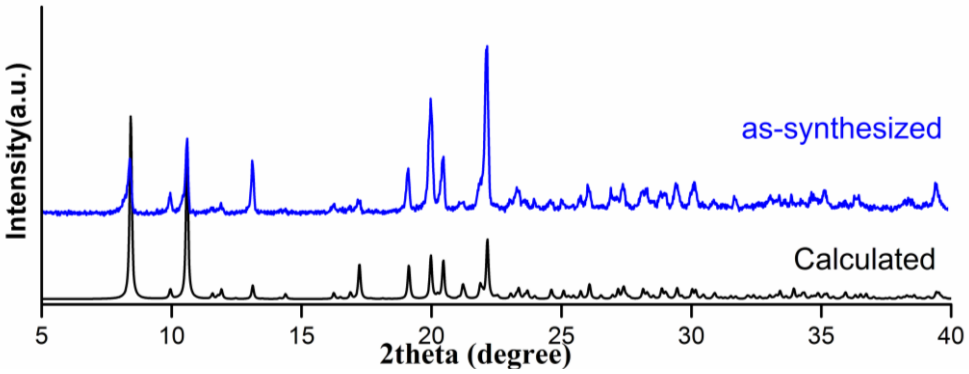

Figure S14. As-synthesized and calculated powder XRD patterns of **14**.

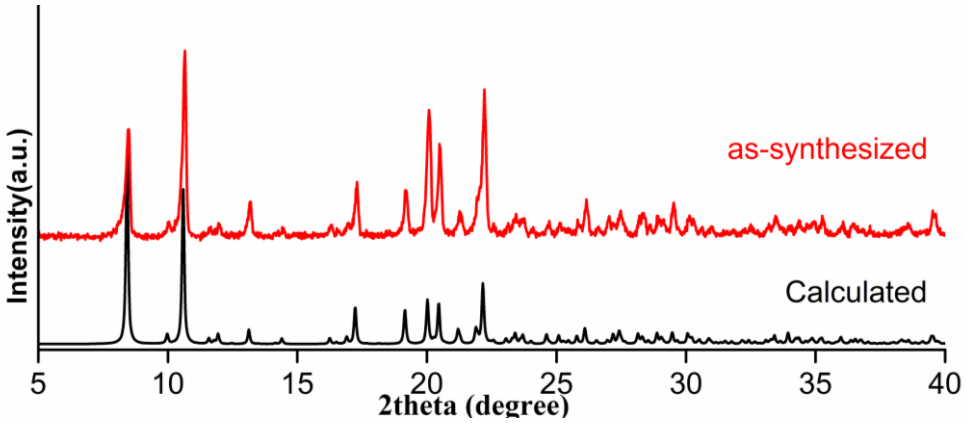

Figure S15. As-synthesized and calculated powder XRD patterns of **15**.

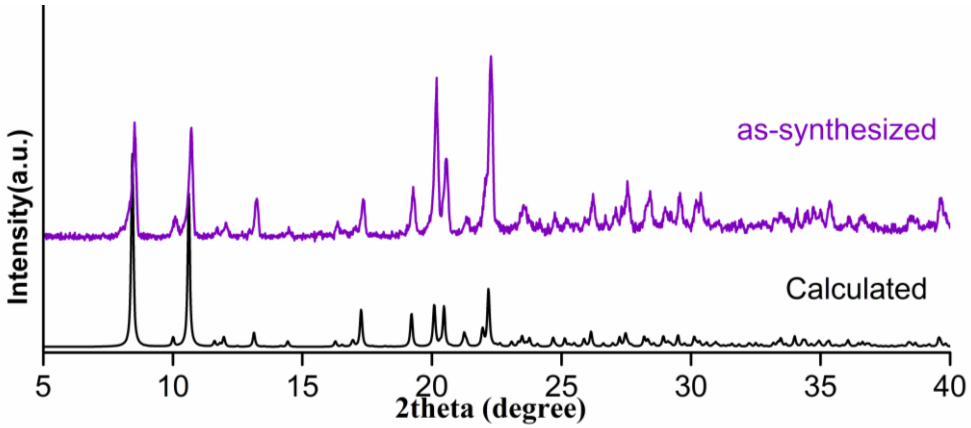

Figure S16. As-synthesized and calculated powder XRD patterns of **16**.

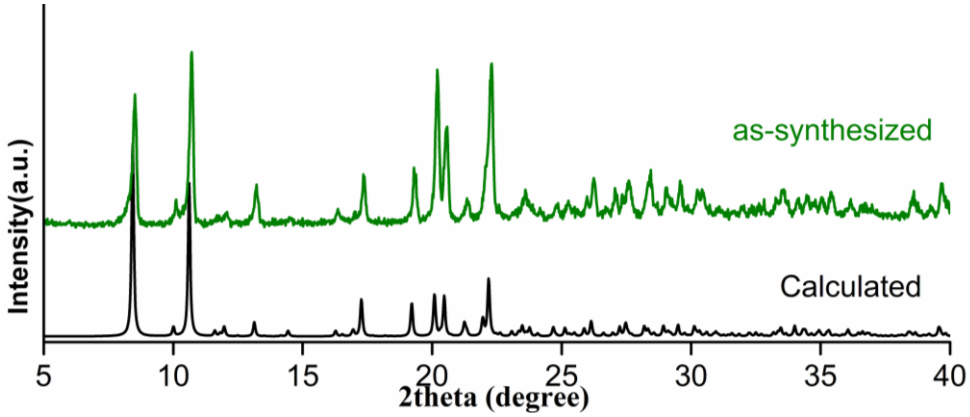

Figure S17. As-synthesized and calculated powder XRD patterns of **17**.

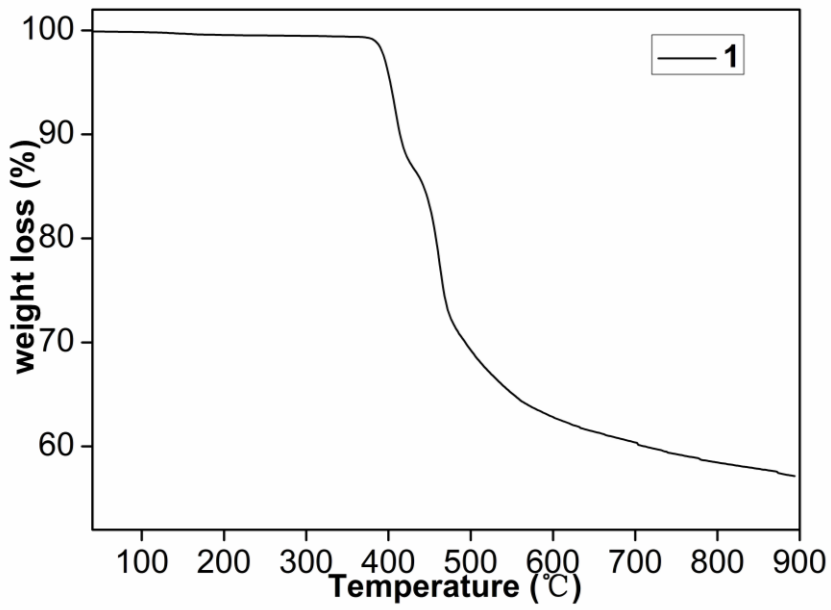

Figure S18. Thermogravimetric analysis (TGA) curve of **1**.

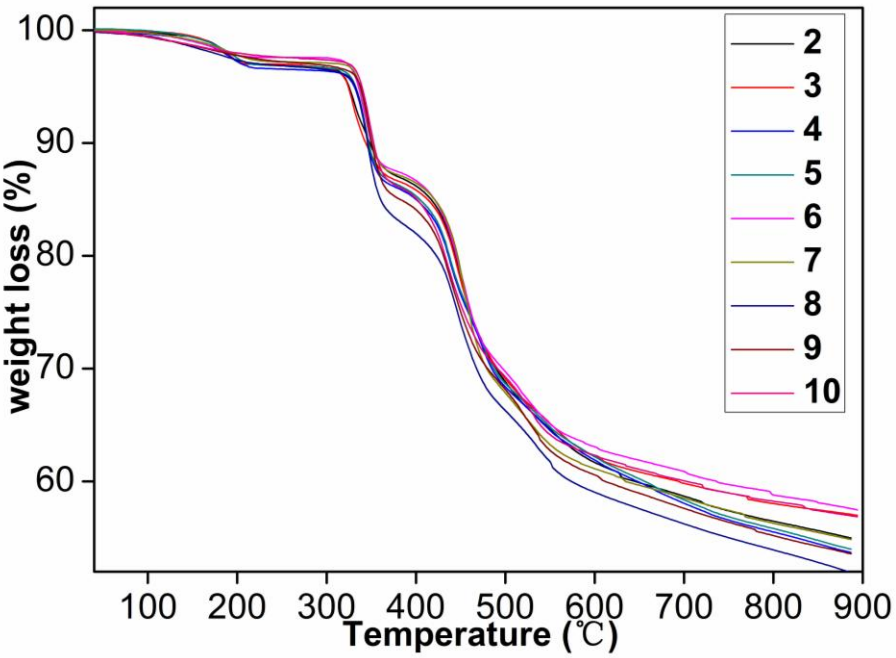

Figure S19. Thermogravimetric analysis (TGA) curves of **2-10**.

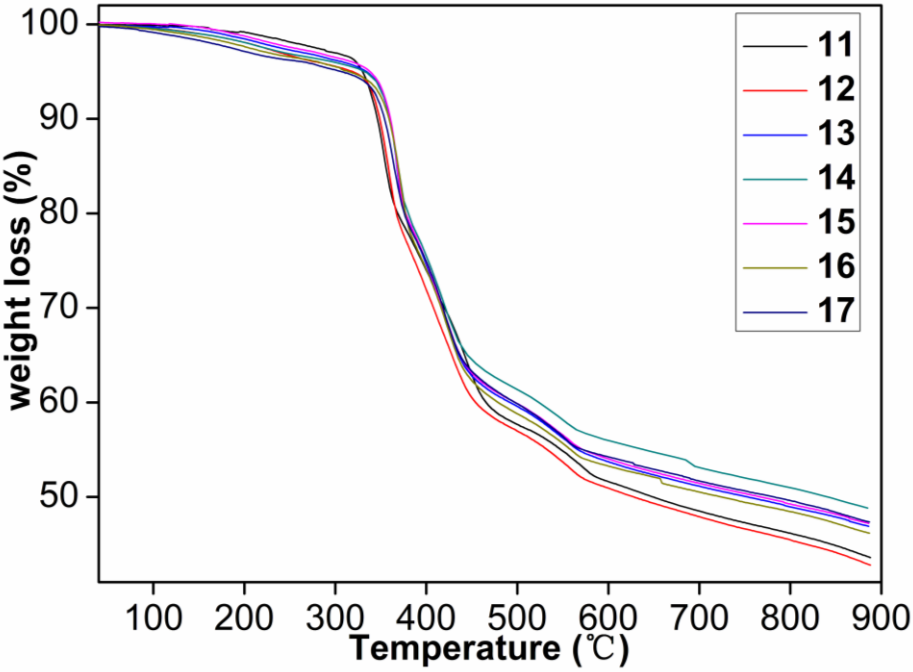

Figure S20. Thermogravimetric analysis (TGA) curves of **11-17**.

Table S1. Selected bond lengths [Å] for compounds **1-17**.

Compound **1**					
La(1)-O(7)#1	2.431(3)	La(1)-O(1)	2.492(3)	La(1)-O(6)	2.538(3)
La(1)-O(8)#1	2.565(3)	La(1)-O(9)	2.571(3)	La(1)-O(4)	2.602(3)
La(1)-O(2)#2	2.607(3)	La(1)-O(8)	2.752(3)	La(1)-O(3)	2.771(3)
Ag(1)-N(1)#3	2.245(4)	Ag(1)-N(2)#4	2.297(4)	Ag(1)-O(4)#5	2.570(3)
Ag(1)-O(2)	2.589(4)				
Compound **2**					
Pr(1)-O(8)#1	2.382(2)	Pr(1)-O(9)#2	2.405(3)	Pr(1)-O(1)#3	2.409(3)
Pr(1)-O(7)#3	2.492(2)	Pr(1)-O(3)#3	2.505(3)	Pr(1)-O(6)	2.525(2)
Pr(1)-O(10)	2.573(3)	Pr(1)-O(2)	2.614(3)	Pr(1)-O(1)	2.644(2)
Ag(1)-N(2)	2.145(3)	Ag(1)-N(1)#1	2.164(3)	Ag(1)-O(2)	2.540(3)
Compound **3**					
Nd(1)-O(9)#1	2.366(3)	Nd(1)-O(8)#2	2.391(3)	Nd(1)-O(1)#3	2.396(3)
Nd(1)-O(6)	2.475(3)	Nd(1)-O(3)#3	2.497(3)	Nd(1)-O(7)#3	2.511(3)
Nd(1)-O(10)	2.560(3)	Nd(1)-O(2)	2.595(3)	Nd(1)-O(1)	2.631(3)
Ag(1)-N(2)	2.155(4)	Ag(1)-N(1)#4	2.163(4)	Ag(1)-O(2)	2.549(3)
Compound **4**					
Sm(1)-O(8)#1	2.336(3)	Sm(1)-O(1)#2	2.360(3)	Sm(1)-O(9)#3	2.367(4)
Sm(1)-O(6)	2.451(4)	Sm(1)-O(3)#2	2.473(4)	Sm(1)-O(7)#2	2.481(4)
Sm(1)-O(10)	2.536(4)	Sm(1)-O(2)	2.563(4)	Sm(1)-O(1)	2.616(3)
Ag(1)-N(2)	2.150(4)	Ag(1)-N(1)#4	2.168(4)	Ag(1)-O(2)	2.555(4)
Compound **5**					
Eu(1)-O(9)#1	2.325(3)	Eu(1)-O(1)#2	2.338(3)	Eu(1)-O(8)#3	2.350(3)
Eu(1)-O(7)#4	2.434(3)	Eu(1)-O(3)#2	2.468(3)	Eu(1)-O(6)#5	2.471(3)
Eu(1)-O(10)	2.521(3)	Eu(1)-O(2)	2.545(3)	Eu(1)-O(1)	2.615(3)
Ag(1)-N(2)	2.157(4)	Ag(1)-N(1)	2.172(4)	Ag(1)-O(2)	2.558(3)
Compound **6**					
Gd(1)-O(9)#1	2.310(3)	Gd(1)-O(1)#2	2.330(3)	Gd(1)-O(8)#3	2.339(3)

Gd(1)-O(6)	2.424(3)	Gd(1)-O(7)#2	2.458(3)	Gd(1)-O(3)#2	2.463(3)
Gd(1)-O(10)	2.508(3)	Gd(1)-O(2)	2.528(3)	Gd(1)-O(1)	2.612(3)
Ag(1)-N(2)	2.151(4)	Ag(1)-N(1)#4	2.169(4)	Ag(1)-O(2)	2.553(3)
Compound **7**					
Tb(1)-O(9)#1	2.298(6)	Tb(1)-O(1)#2	2.318(7)	Tb(1)-O(8)#3	2.343(7)
Tb(1)-O(6)	2.398(7)	Tb(1)-O(7)#2	2.441(7)	Tb(1)-O(3)#2	2.462(8)
Tb(1)-O(10)	2.507(8)	Tb(1)-O(2)	2.512(8)	Tb(1)-O(1)	2.610(7)
Ag(1)-N(2)	2.158(8)	Ag(1)-N(1)#4	2.178(8)	Ag(1)-O(2)	2.562(7)
Compound **8**					
Dy(1)-O(8)#1	2.262(3)	Dy(1)-O(1)#2	2.284(3)	Dy(1)-O(9)#3	2.323(3)
Dy(1)-O(6)	2.378(3)	Dy(1)-O(7)#2	2.411(3)	Dy(1)-O(2)	2.467(4)
Dy(1)-O(3)#2	2.518(4)	Dy(1)-O(10)	2.541(4)	Dy(1)-O(1)	2.603(3)
Ag(1)-N(2)	2.163(4)	Ag(1)-N(1)#4	2.178(4)	Ag(1)-O(2)	2.637(4)
Compound **9**					
Ho(1)-O(8)#1	2.249(3)	Ho(1)-O(1)#2	2.274(3)	Ho(1)-O(9)#3	2.304(3)
Ho(1)-O(7)#2	2.366(3)	Ho(1)-O(6)	2.399(3)	Ho(1)-O(2)	2.459(4)
Ho(1)-O(3)#2	2.516(4)	Ho(1)-O(10)	2.538(4)	Ho(1)-O(1)	2.599(3)
Ag(1)-N(2)	2.167(4)	Ag(1)-N(1)#1	2.173(4)	Ag(1)-O(2)	2.642(4)
Compound **10**					
Er(1)-O(9)#1	2.242(3)	Er(1)-O(1)#2	2.251(4)	Er(1)-O(8)#3	2.289(4)
Er(1)-O(7)	2.348(4)	Er(1)-O(6)#2	2.382(3)	Er(1)-O(2)	2.434(4)
Er(1)-O(3)#2	2.517(4)	Er(1)-O(10)	2.530(4)	Er(1)-O(1)	2.599(3)
Ag(1)-N(2)	2.165(5)	Ag(1)-N(1)#4	2.173(4)	Ag(1)-O(2)	2.649(4)
Compound **11**					
La(1)-O(8)#1	2.435(2)	La(1)-O(9)#2	2.448(2)	La(1)-O(1)#3	2.472(2)
La(1)-O(3)#3	2.535(2)	La(1)-O(6)	2.539(2)	La(1)-O(7)#3	2.540(2)
La(1)-O(10)	2.586(2)	La(1)-O(1)	2.675(2)	La(1)-O(2)	2.692(2)
Cu(1)-N(2)	1.904(3)	Cu(1)-N(1)#4	1.911(3)	Cu(1)-O(2)	2.354(2)
Compound **12**					

Pr(1)-O(8)#1	2.391(2)	Pr(1)-O(9)#2	2.408(3)	Pr(1)-O(1)#3	2.427(2)
Pr(1)-O(3)#3	2.494(2)	Pr(1)-O(6)	2.496(3)	Pr(1)-O(7)#3	2.500(3)
Pr(1)-O(10)	2.555(3)	Pr(1)-O(2)	2.641(2)	Pr(1)-O(1)	2.645(2)
Cu(1)-N(2)	1.897(3)	Cu(1)-N(1)#1	1.909(3)	Cu(1)-O(2)	2.364(3)
Compound **13**					
Nd(1)-O(8)#1	2.375(3)	Nd(1)-O(9)#2	2.395(4)	Nd(1)-O(1)#3	2.411(3)
Nd(1)-O(3)#3	2.483(4)	Nd(1)-O(6)	2.485(4)	Nd(1)-O(7)#3	2.489(3)
Nd(1)-O(10)	2.529(4)	Nd(1)-O(2)	2.624(3)	Nd(1)-O(1)	2.628(3)
Cu(1)-N(2)	1.907(4)	Cu(1)-N(1)#1	1.909(4)	Cu(1)-O(2)	2.367(3)
Compound **14**					
Sm(1)-O(8)#1	2.340(2)	Sm(1)-O(9)#2	2.371(3)	Sm(1)-O(1)#3	2.377(2)
Sm(1)-O(7)#3	2.458(3)	Sm(1)-O(6)	2.458(3)	Sm(1)-O(3)#3	2.461(3)
Sm(1)-O(10)	2.510(3)	Sm(1)-O(2)	2.594(3)	Sm(1)-O(1)	2.616(2)
Cu(1)-N(2)	1.899(3)	Cu(1)-N(1)#1	1.916(3)	Cu(1)-O(2)	2.381(3)
Compound **15**					
Eu(1)-O(8)#1	2.336(4)	Eu(1)-O(9)#2	2.358(4)	Eu(1)-O(1)#3	2.366(4)
Eu(1)-O(7)#3	2.443(4)	Eu(1)-O(6)	2.454(4)	Eu(1)-O(3)#3	2.461(4)
Eu(1)-O(10)	2.503(4)	Eu(1)-O(2)	2.575(4)	Eu(1)-O(1)	2.613(3)
Cu(1)-N(2)	1.903(5)	Cu(1)-N(1)#1	1.916(5)	Cu(1)-O(2)	2.390(4)
Compound **16**					
Gd(1)-O(8)#1	2.318(3)	Gd(1)-O(9)#2	2.343(3)	Gd(1)-O(1)#3	2.350(3)
Gd(1)-O(7)#3	2.429(3)	Gd(1)-O(6)	2.439(3)	Gd(1)-O(3)#3	2.447(3)
Gd(1)-O(10)	2.489(4)	Gd(1)-O(2)	2.557(3)	Gd(1)-O(1)	2.607(3)
Cu(1)-N(2)	1.902(4)	Cu(1)-N(1)#1	1.915(4)	Cu(1)-O(2)	2.397(3)
Compound **17**					
Tb(1)-O(8)#1	2.314(6)	Tb(1)-O(9)#2	2.333(7)	Tb(1)-O(1)#3	2.337(6)
Tb(1)-O(6)	2.419(6)	Tb(1)-O(7)#3	2.429(7)	Tb(1)-O(3)#3	2.439(7)
Tb(1)-O(10)	2.472(7)	Tb(1)-O(2)	2.547(7)	Tb(1)-O(1)	2.606(6)
Cu(1)-N(2)	1.906(8)	Cu(1)-N(1)#1	1.911(8)	Cu(1)-O(2)	2.404(7)

Symmetry codes: For **1** #1 x,-y+3/2,z+1/2 #2 x,-y+3/2,z-1/2 #3 -x,-y+2,-z+1 #4 x+1,-y+3/2,z+3/2 #5 x,y,z+1.

2 #1 x-1/2,-y+1/2,z-1/2 #2 -x+1/2,y+1/2,-z+1/2 #3 -x+1,-y+1,-z.

3 #1 x-1/2,-y+1/2,z-1/2 #2 -x+1/2,y-1/2,-z+1/2 #3 -x+1,-y,-z #4 -x+1/2,y+1/2,-z-1/2.

4 #1 x-1/2,-y+3/2,z-1/2 #2 -x+2,-y+2,-z #3 -x+3/2,y+1/2,-z+1/2 #4 -x+3/2,y-1/2,-z-1/2.

5 #1 x+1/2,-y+3/2,z+1/2. #2 -x+1,-y+2,-z+1. #3 -x+3/2,y+1/2,-z+1/2. #4 -x+3/2,y+1/2,-z+3/2.

6 #1 x+1/2,-y+1/2,z+1/2 #2 -x+1,-y+1,-z #3 -x+3/2,y+1/2,-z-1/2 #4 -x+3/2,y-1/2,-z+1/2.

7 #1 x-1/2,-y+1/2,z-1/2 #2 -x+1,-y+1,-z #3 -x+1/2,y+1/2,-z+1/2 #4 -x+1/2,y-1/2,-z-1/2.

8 #1 x+1/2,-y+1/2,z+1/2 #2 -x+1,-y+1,-z #3 -x+3/2,y+1/2,-z-1/2 #4 -x+3/2,y-1/2,-z+1/2.

9 #1 x-1/2,-y+3/2,z-1/2 #2 -x+2,-y+1,-z+2 #3 -x+3/2,y-1/2,-z+5/2.

10 #1 x+1/2,-y+1/2,z+1/2 #2 -x+1,-y,-z #3 -x+3/2,y-1/2,-z-1/2 #4 -x+3/2,y+1/2,-z+1/2.

11 #1 x+1/2,-y+3/2,z+1/2. #2 -x+3/2,y+1/2,-z+1/2. #3 -x+1,-y+2,-z+1. #4 -x+3/2,y-1/2,-z+3/2.

12 #1 x+1/2,-y+5/2,z+1/2 #2 -x+5/2,y-1/2,-z-1/2 #3 -x+2,-y+2,-z.

13 #1 x-1/2,-y+5/2,z-1/2 #2 -x+1/2,y-1/2,-z+3/2 #3 -x+1,-y+2,-z+1.

14 #1 x+1/2,-y+3/2,z+1/2 #2 -x+3/2,y+1/2,-z+1/2 #3 -x+1,-y+2,-z+1.

15 #1 x+1/2,-y+3/2,z+1/2 #2 -x+3/2,y+1/2,-z+1/2 #3 -x+1,-y+2,-z+1.

16 #1 x+1/2,-y+3/2,z+1/2 #2 -x+3/2,y+1/2,-z+1/2 #3 -x+1,-y+2,-z+1.

17 #1 x+1/2,-y+3/2,z+1/2 #2 -x+3/2,y+1/2,-z+1/2 #3 -x+1,-y+2,-z+1.