Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

A series of 3d-4f heterometallic coordination polymers constructed from size-tunable copper halide clusters and lanthanide-organic motifs

Guo Peng,[a] Zhihui Liu,[a] Li Ma,[a] Li Liang,[a] Limin Zhang,[a] Hong Deng,*[a] George E Kostakis,*[b]

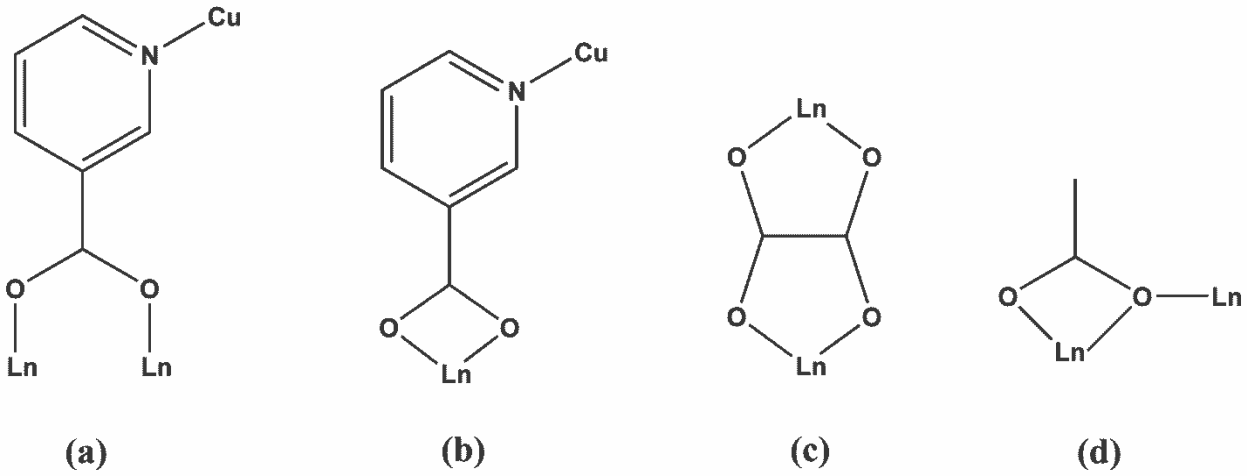
a School of Chemistry & Environment and Key Laboratory of Electrochemical Technology on Energy Storage and Power Generation in Guangdong Universities, South China Normal University, Guangzhou 510006, P. R. China

b Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

**To whom Correspondence should be addressed. E-mail: dh@scnu.edu.cn, George.Kostakis@kit.edu*

Table S1. Selected bond lengths (Å) for compounds **1, 4** and **8-10**

Compound 1					
Sm(1)-O(6)	2.339(6)	Sm(1)-O(8)#1	2.339(7)	Sm(1)-O(12)#2	2.365(6)
Sm(1)-O(2)#3	2.382(6)	Sm(1)-O(3)#4	2.420(7)	Sm(1)-O(10)#4	2.482(7)
Sm(1)-O(1W)	2.507(8)	Sm(1)-O(9)#4	2.630(7)	Sm(2)-O(5)	2.339(6)
Sm(2)-O(11)#2	2.348(6)	Sm(2)-O(4)#2	2.370(6)	Sm(2)-O(7)#5	2.391(7)
Sm(2)-O(1)	2.403(6)	Sm(2)-O(3W)	2.493(7)	Sm(2)-O(2W)	2.535(7)
Sm(2)-O(4W)	2.546(8)	Cu(1)-Br(1)	2.360(2)	Cu(2)-Br(1)	2.403(2)
Cu(1)-Br(2)	2.360(2)	Cu(2)-Br(2)#6	2.499(2)	Cu(2)-Br(2)	2.888(2)
Cu(4)-Br(3)	2.383(2)	Cu(3)-Br(3)	2.543(2)	Cu(6)-Br(3)	2.573(2)
Cu(6)-Br(4)	2.428(2)	Cu(3)-Br(4)	2.439(2)	Cu(4)-Br(5)	2.398(2)
Cu(5)-Br(5)	2.418(2)	Cu(5)-Br(6)	2.412(2)	Cu(6)-Br(6)	2.620(3)
Symmetry codes: #1 -x+2, -y+1, -z+1 #2 x-1, y+1, z #3 x+1, y, z #4 x, y+1, z #5 -x+1, -y+1, -z+1 #6 -x+1, -y+1, -z					
Compound 4					
Cu(2)-Br(1)	2.451(2)	Cu(1)-Br(1)#1	2.552(3)	Cu(1)-Br(1)#2	2.626(3)
Cu(2)-Br(2)	2.383(3)	Cu(1)-Br(2)#1	2.418(3)	Gd(1)-O(1)	2.307(7)
Gd(1)-O(3)	2.340(6)	Gd(1)-O(5)	2.490(6)	Gd(1)-O(6)#3	2.498(6)
Gd(2)-O(4)	2.335(7)	Gd(2)-O(2)#4	2.371(7)	Gd(2)-O(3W)	2.463(7)
Gd(2)-O(4W)	2.485(7)				
Symmetry codes: #1 -x-1/2, y+1/2, z #2 x+1/2, y+1/2, -z+1/2 #3 -x, -y, -z+1 #4 -x, y, -z+1/2					
Compound 8					
Cu(3)-Br(1)#1	2.312(3)	Cu(2)-Br(1)	2.405(3)	Cu(1)-Br(1)	2.653(4)
Cu(3)-Br(2)	2.506(3)	Cu(1)-Br(2)	2.583(3)	Cu(2)-Br(3)#1	2.337(3)
Cu(1)-Br(3)	2.400(3)	Tb(1)-O(1)	2.317(10)	Tb(1)-O(2)#2	2.288(10)
Tb(1)-O(3)	2.385(11)	Tb(1)-O(4)#3	2.348(10)	Tb(1)-O(4)	2.473(10)
Tb(1)-O(5)	2.280(10)	Tb(1)-O(6)#3	2.312(10	Tb(1)-O(1W)	2.381(11)
Symmetry codes: #1 -x+1, -y+2, -z+1 #2 x, -y+3/2, z+1/2 #3 -x+2, -y+2, -z					
Compound 9					
Cu(1)-Br(1)	2.431(2)	Cu(1)-Br(2)	2.576(2)	Cu(1)-Br(3)	2.669(2)
Cu(2)-Br(2)	2.399(2)	Cu(2)-Br(1)	2.401(2)	Cu(3)-Br(6)	2.323(7)
Cu(3)-Br(4)	2.451(4)	Cu(3)-Br(2)#1	2.537(3)	Cu(3)-Br(3)	2.785(3)
Cu(4)-Br(4)#1	2.176(8)	Cu(4)-Br(1)#1	2.537(7)	Er(1)-O(2)#2	2.227(8)
Er(1)-O(3)	2.269(7)	Er(1)-O(1W)	2.423(9)	Er(1)-O(2W)	2.479(7)
Er(2)-O(1)#3	2.248(7)	Er(2)-O(4)	2.266(6)	Er(2)-O(6)	2.431(7)
Er(2)-O(5)	2.446(7)				
Symmetry codes: #1 -x+1/2, y, -z+3/2 #2 x+1/2, -y+1, z-1/2 #3 -x+1, -y+2, -z+2					
Compound 10					
Cu(2)-Cl(1)	2.327(3)	Cu(1)-Cl(1)	2.488(2)	Cu(3)-Cl(2)#1	2.215(2)
Cu(2)-Cl(2)	2.234(3)	Cu(2)-Cl(3)	2.247(3)	Cu(3)-Cl(3)#2	2.482(3)
Gd(1)-O(3)#3	2.323(5)	Gd(1)-O(2)#1	2.326(5)	Gd(1)-O(6)#4	2.379(5)
Gd(1)-O(5)	2.381(5)	Gd(1)-O(4)#5	2.383(5)	Gd(1)-O(1)	2.387(5)
Gd(1)-O(2W)	2.476(5)	Gd(1)-O(1W)	2.551(5)		
Symmetry codes: #1 -x+1, -y+1, -z+1 #2 x, -y+1/2, z-1/2 #3 x, y+1, z #4 -x, -y+1, -z+1 #5 -x, -y, -z+1					



Scheme S1 Coordination modes of nicotinate, oxalate, acetate ligands in compounds **1**-**10**.

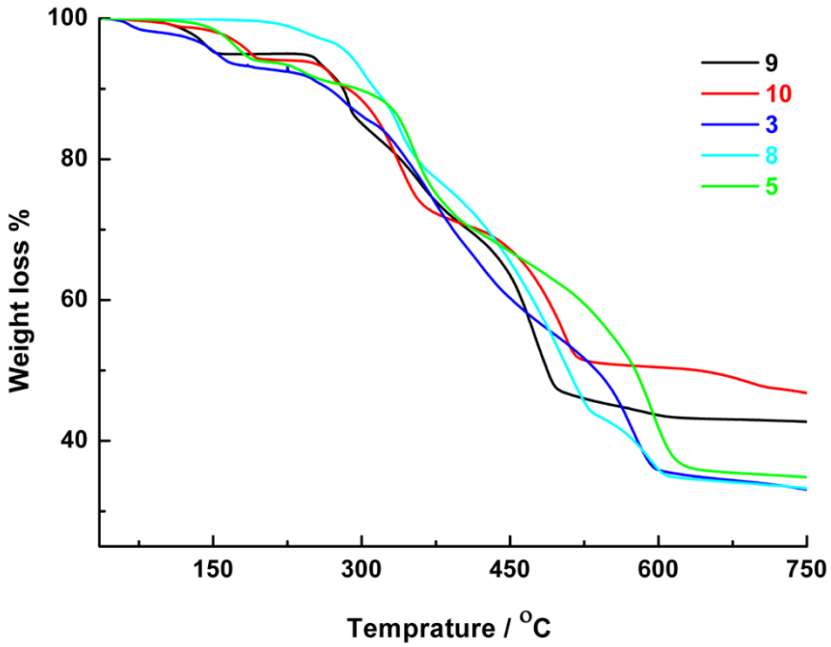


Fig. S1. The TGA curves of compounds **3**, **5**, **8**, **9** and **10**

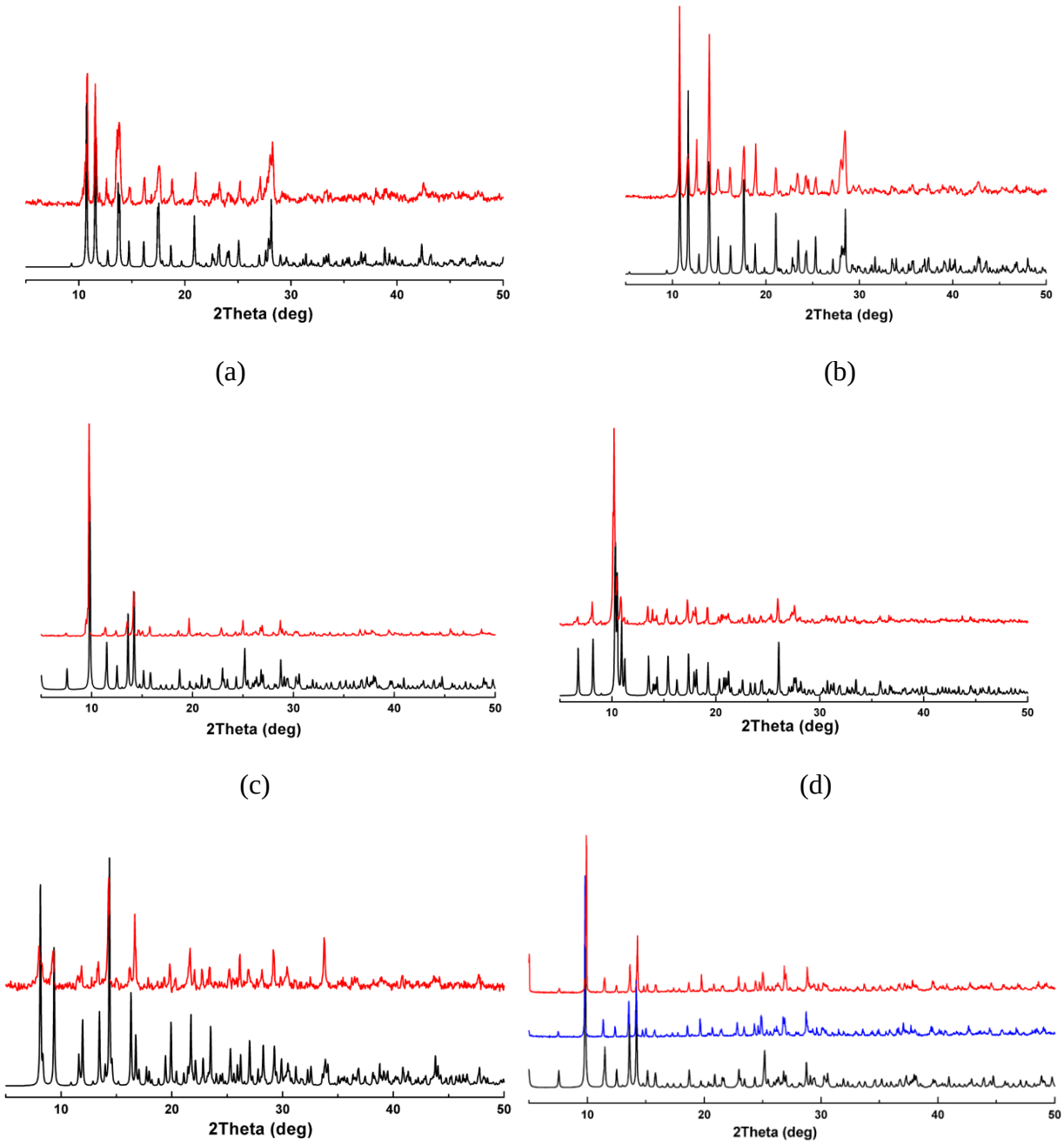
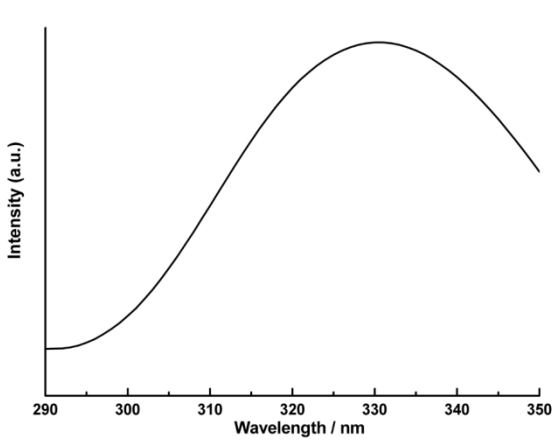
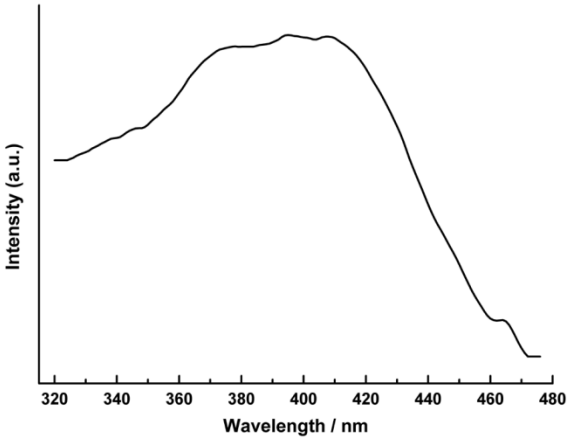


Fig. S2 PXRD patterns for: (a) compound **4**, as simulated (black) and as synthesized (red); (b) compound **5**, as simulated (black) and as synthesized (red); (c) compound **8**, as simulated (black) and as synthesized (red); (d) compound **9**, as simulated (black) and as synthesized (red); (e)

compound **10**, as simulated (black) and as synthesized (red); (f) compounds **6-7**, as simulated for **8** (black) and as synthesized for **6** (bule) and **7** (red).



(a)



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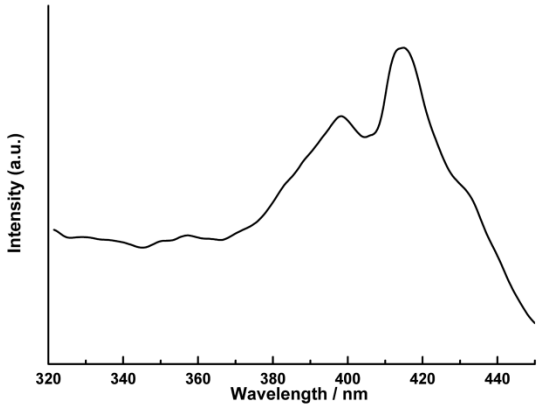
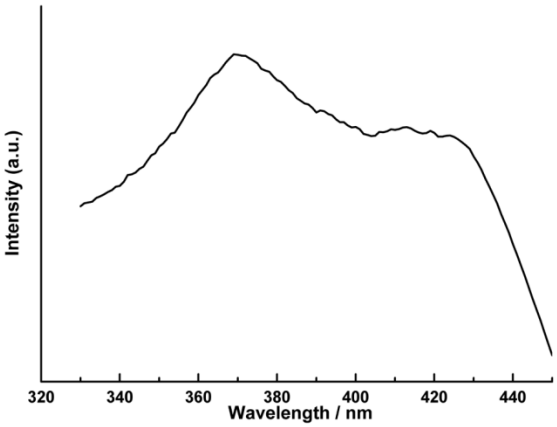
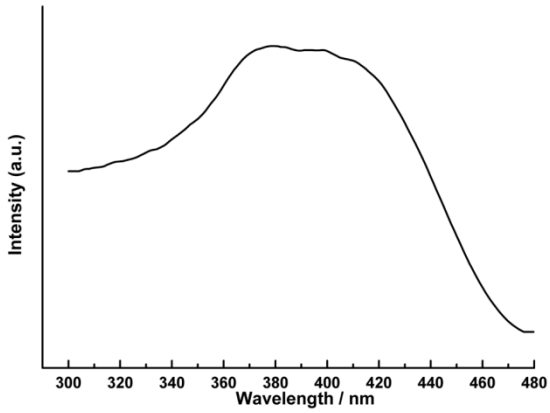


(c)

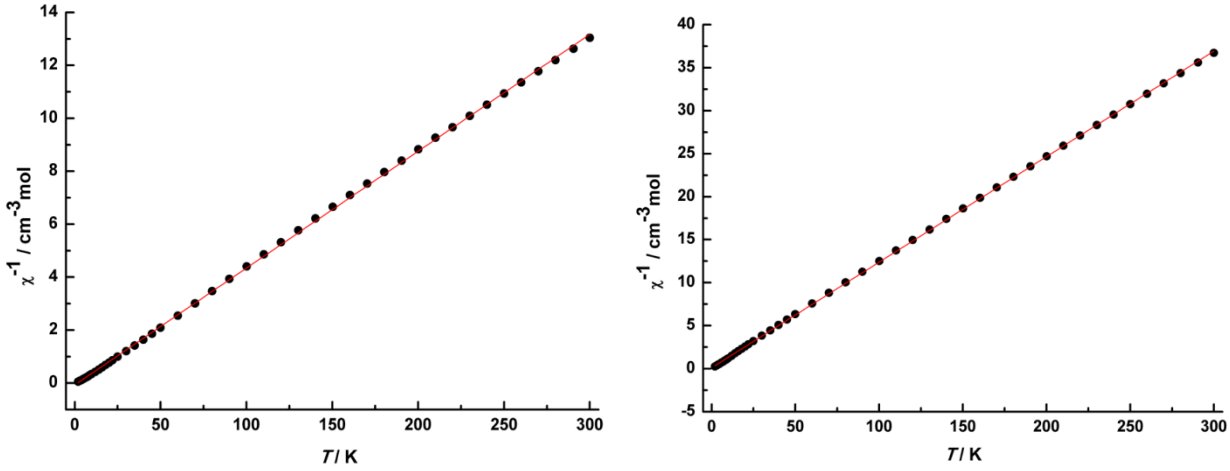


(d)



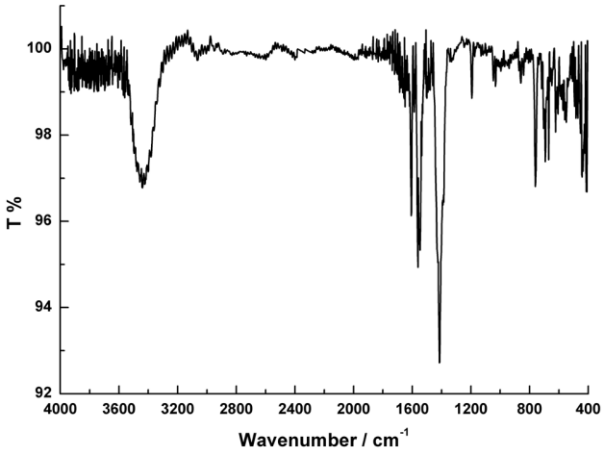
(e)

Fig. S3 The excitation spectra for (a) HNA ligand, (b) compound **1**, (c) compound **3**, (d) compound **6**, (e) compound **8**.

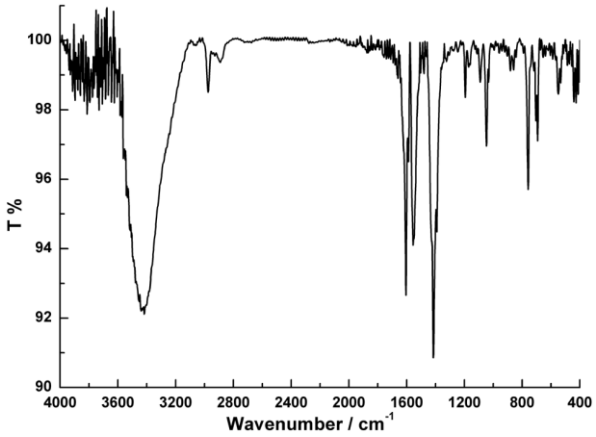


(a) (b)

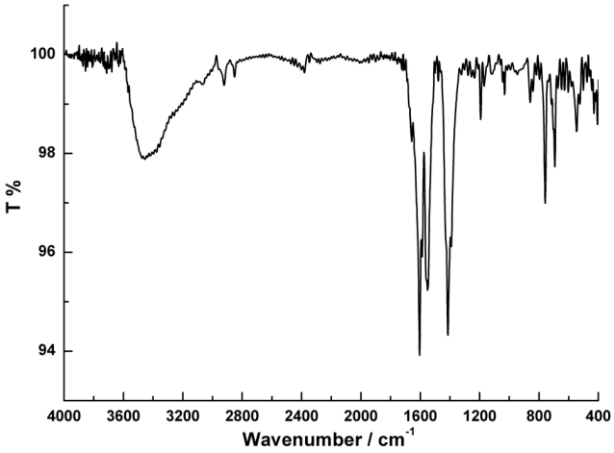
Fig. S4 The temperature dependence of χ^{-1} curves for compound **9** (a) and **10** (b).



(1)



(2)



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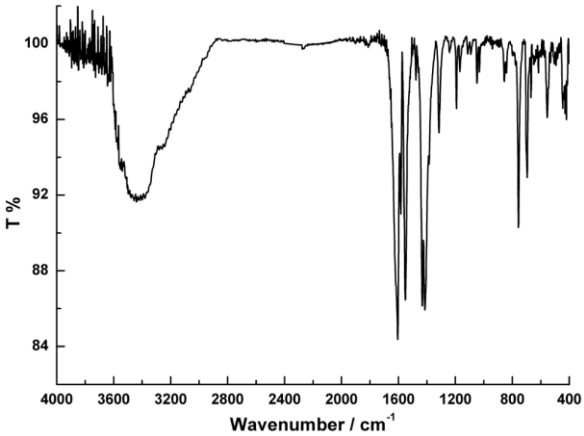

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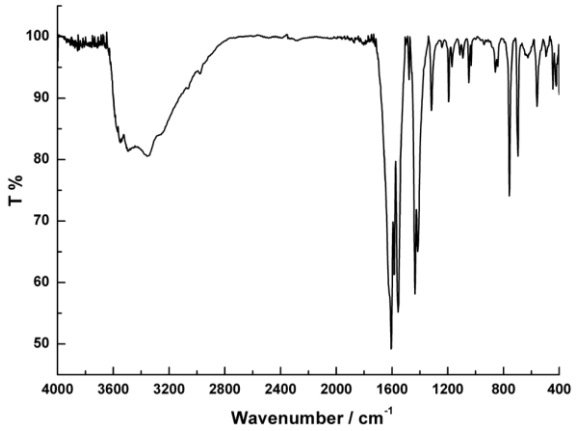

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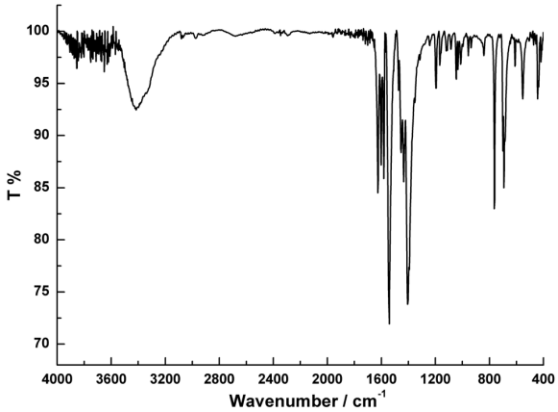
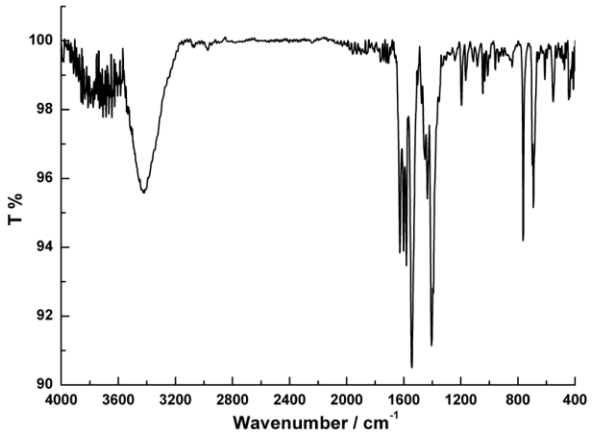
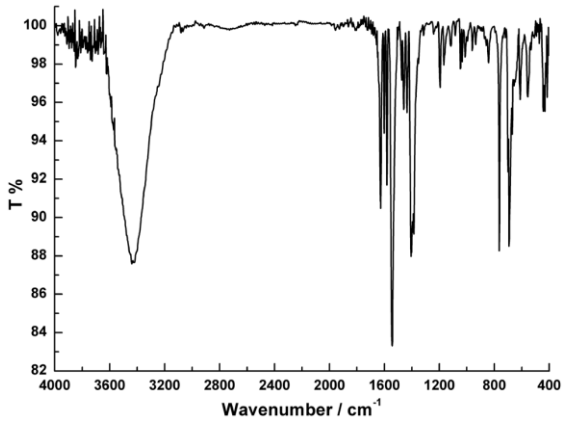


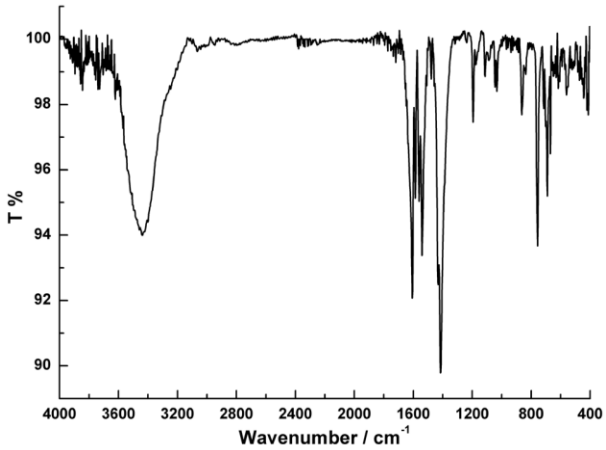
(6)



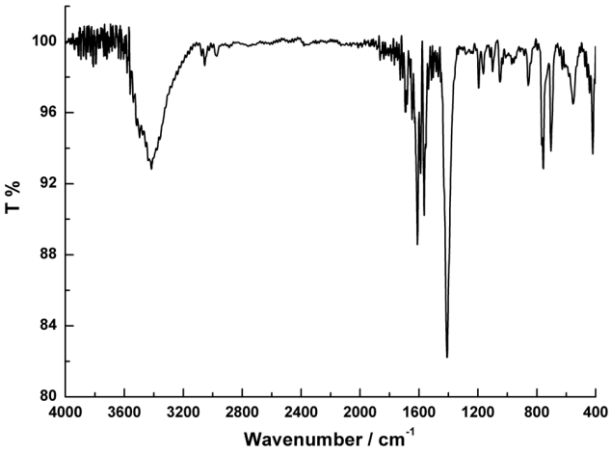
(7)



(8)



(9)



(10)

Fig. S5 IR plots of compounds **1-10**.