Electronic supplementary information (ESI)

Direct Assembly of New Cobalt(III)-Lanthanide(III) Heterometallic

Frameworks with NaCl-like Topology

Hai-Yang Liu,^a Yong-Jun Yuan,^{a,b} Zhen-Tao Yu*^{a,b} and Zhi-Gang Zou^a

 ^aEco-Materials and Renewable Energy Research Center, National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China. Fax: (+86) 25-83686632. E-mail: yuzt@nju.edu.cn
 ^bDepartment of Materials Science and Engineering, Nanjing University, Nanjing 210093, China



Fig. S1. The XPS spectra for compounds 1 and 2.



Fig. S2. Powder X-ray diffraction (PXRD) patterns of 1.



Fig. S3. Powder X-ray diffraction (PXRD) patterns simulated and experimental of **2** and **2**' (after dehydration).

Supplementary Material (ESI) for CrystEngComm This journal is (c) The Royal Society of Chemistry 2011



Fig. S4. Powder X-ray diffraction (PXRD) patterns of 2-5 from prepared samples.



Fig. S5 View of the chain packing for **1** along the [100] direction (left); the extended structure of **1** viewed along the [001] direction (right). The noncoordinating water molecules occluded in the channels and all hydrogen atoms are omitted for clarity.



Fig. S6. χ_M vs T plot for compound **2**.



Fig. S7. The TGA curves for compounds 2-5.

	1		
Co1-N3	1.923(3)	Co1-N4	1.913(3)
Co1-N5	1.929(3)	Co1-N6	1.924(3)
Co1-N7	1.923(3)	Co1-N8	1.952(3)
Co2-N1	2.126(3)	Co2-N2	2.128(3)
Co2-O6	2.088(2)	Co2-O13	2.067(2)
Co2-O1w	2.107(2)	Co2-O2w	2.162(3)
N3-Co1-N4	82.90(13)	N5-Co1-N6	83.56(13)
N7-Co1-N8	83.69(13)	N3-Co1-N5	95.36(13)
N3-Co1-N7	87.66(13)	N5-Co1-N8	93.14(12)
N1-Co2-N2	76.14(11)	N1-Co2-O1w	89.41(10)
O6-Co-O2w	91.06(9)	O6-Co2-O13	91.17(10)
	2		
Co1-N1	1.858(5)	Co1-N2	1.920(5)
Co1-N3	1.917(4)	Co1-N4	1.902(5)
Co1-N5	1.950(5)	Co1-N6	1.943(5)
Gd1-O1	2.269(4)	Gd1-O2	2.283(4)
Gd1-O10	2.285(4)	Gd1-O11	2.410(5)
Gd1-O12	2.271(4)	Gd1-O1w	2.456(4)
Gd1-O2w	2.377(5)	Gd1-O3w	2.416(4)
Gd2-O3	2.374(4)	Gd2-O4	2.314(4)
Gd2-O5	2.338(4)	Gd2-O7	2.331(4)
Gd2-O8	2.394(4)	Gd2-O4w	2.427(4)

 Table S1. Selected bond lengths and angles for compounds 1-5.

Supplementary Material (ESI) for CrystEngComm	
This journal is (c) The Royal Society of Chemistry 201	1

Gd2-O5w	2.381(4)	Gd2-O6w	2.446(5)
N1-Co1-N2	84.1(2)	N1-Co1-N4	91.2(2)
N2-Co1-N5	178.0(2)	N4-Co1-N6	178.1(2)
O1-Gd1-O10	85.46(16)	O1-Gd1-O2	119.05(17)
O2-Gd1-O2w	74.98(16)	O2w-Gd1-O3w	72.80(17)
O4-Gd2-O5	76.81(15)	O7-Gd2-O8	120.61(15)
O5-Gd2-O6w	75.33(16)	O4w-Gd2-O5w	70.08(17)
	3		
Co1-N1	1.874(4)	Co1-N2	1.924(4)
Co1-N3	1.942(4)	Co1-N4	1.916(4)
Co1-N5	1.954(4)	Co1-N6	1.947(4)
Eu1-O1	2.277(3)	Eu1-O2	2.305(4)
Eu1-O10	2.291(3)	Eu1-O11	2.421(4)
Eu1-O12	2.286(3)	Eu1-O1w	2.476(4)
Eu1-O2w	2.396(4)	Eu1-O3w	2.429(4)
Eu2-O3	2.380(4)	Eu2-O4	2.319(4)
Eu2-O5	2.347(4)	Eu2-O7	2.346(3)
Eu2-O8	2.399(4)	Eu2-O4w	2.441(4)
Eu2-O5w	2.386(4)	Eu2-O6w	2.454(4)
N1-Co1-N2	84.14(19)	N1-Co1-N4	91.38(19)
N2-Co1-N5	177.64(19)	N4-Co1-N6	177.53(18)
O1-Eu1-O10	85.18(13)	O1-Eu1-O2	119.14(13)
O2-Eu1-O2w	74.97(13)	O2w-Eu1-O3w	72.41(14)
O4-Eu2-O5	76.89(12)	O7-Eu2-O8	120.61(12)
O5-Eu2-O6w	75.14(13)	O4w-Eu2-O5w	69.91(14)
4			
Co1-N1	1.875(4)	Co1-N2	1.924(4)

Supplementary Material (ESI) for CrystEngComm	
This journal is (c) The Royal Society of Chemistry 20)11

Co1-N3	1.940(3)	Co1-N4	1.908(4)
Col-N5	1.962(4)	Col-N6	1.964(3)
Sm1-O1	2.288(4)	Sm1-O2	2.309(4)
Sm1-O10	2.294(4)	Sm1-O11	2.430(4)
Sm1-O12	2.285(4)	Sm1-O1w	2.467(4)
Sm1-O2w	2.397(4)	Sm1-O3w	2.439(4)
Sm2-O3	2.391(4)	Sm2-O4	2.331(4)
Sm2-O5	2.352(4)	Sm2-O7	2.344(4)
Sm2-O8	2.414(4)	Sm2-O4w	2.441(4)
Sm2-O5w	2.400(4)	Sm2-O6w	2.460(4)
N1-Co1-N2	84.3(2)	N1-Co1-N4	91.3(2)
N2-Co1-N5	177.8(2)	N4-Co1-N6	177.9(2)
O1-Sm1-O10	85.29(14)	O1-Sm1-O2	118.85(14)
O2-Sm1-O2w	75.17(14)	O2w-Sm1-O3w	72.82(14)
O4-Sm2-O5	76.96(13)	O7-Sm2-O8	120.77(13)
O5-Sm2-O6w	75.53(13)	O4w-Sm2-O5w	69.93(14)
	5		
Col-N1	1.869(4)	Co1-N2	1.925(5)
Co1-N3	1.938(4)	Col-N4	1.925(5)
Col-N5	1.959(4)	Col-N6	1.960(4)
La1-O1	2.304(4)	La1-O2	2.308(4)
La1-O10	2.294(4)	La1-O11	2.459(4)
La1-O12	2.282(4)	La1-O1w	2.523(4)
La1-O2w	2.393(4)	La1-O3w	2.395(4)
La2-O3	2.404(4)	La2-O4	2.339(4)
La2-O5	2.326(4)	La2-O7	2.351(4)
La2-O8	2.404(4)	La2-O4w	2.488(4)

Supplementary Material (ESI) for CrystEngComm This journal is (c) The Royal Society of Chemistry 2011

La2-O5w	2.356(4)	La2-O6w	2.478(4)
N1-Co1-N2	85.5(2)	N1-Co1-N4	91.0(2)
N2-Co1-N5	178.1(2)	N4-Co1-N6	178.0(2)
O1-La1-O10	85.77(14)	O1-La1-O2	119.60(15)
O2-La1-O2w	73.54(15)	O2w-La1-O3w	74.00(15)
O4-La2-O5	77.79(13)	O7-La2-O8	120.14(13)
O5-La2-O6w	75.54(15)	O4w-La2-O5w	69.47(15)

Symmetry code: (i) -1+x, y, z; (ii) 1+x, y, z For 1. (i) 1-x, 2-y, 1-z; (ii) 2-x, 2-y, 1-z; (iii) 1-x, 1-y, 1-z; (iv) x, -1+y, z; (v) -x, 1-y, -z; (vi) 1-x, 1-y, -z; (vii) -1+x, -1+y, z; (viii) -1+x, y, z; (ix) 1+x, 1+y, z; (x) 1+x, y, z; (xi) x, 1+y, z for 2-5