Supplementary information (ESI) for *CrystEngComm*

Supplementary Materials

Nanosized lanthanide oxide rods in I^1O^3 hybrid organic-inorganic frameworks involving *in situ* ligand synthesis

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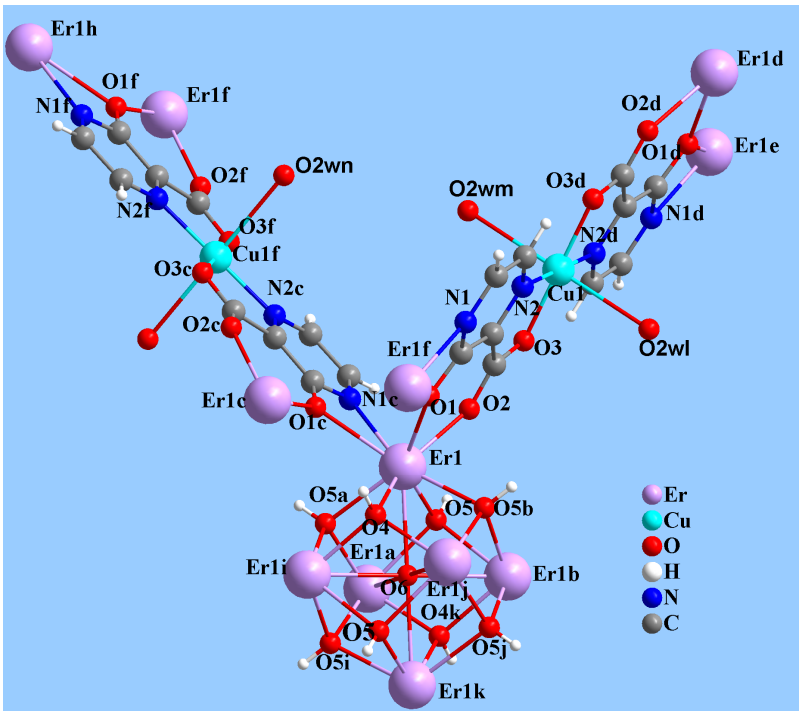

Figure S1. The coordination environments of Er1 and Cu1 atoms in **3**, Er_6 cluster constructed by Er1 atom and each Er1 atom bridged by two L^{Cu} SBUs. Atom label with "a" or "b", etc. refer to symmetry-generated atoms. Symmetry codes: (a) 1/3+y, 2/3-x+y, 2/3-z; (b) 1/3+x-y, -1/3+x, 2/3-z; (c) 1/3+y, 2/3-x+y, -1/3-z; (d) 2-x, 1-y, -z; (e) 5/3-x +y, 4/3-x, 1/3+z; (f) 1/3+x-y, -1/3+x, -1/3-z; (g) 4/3-y, -1/3+x-y, -1/3+z; (h) 5/3-x, 1/3-y, -2/3-z; (i) 1-x+y, 1-x, z; (j) 1-y, x-y, z; (k) 4/3-x, 2/3-y, 2/3-z; (l) x, y, 1+z; (m) 2-x, 1-y, 1-z; (n) 1/3+y, 2/3-x+y, -4/3-z; (o) 4/3-y, -1/3+x-y, 2/3+z.

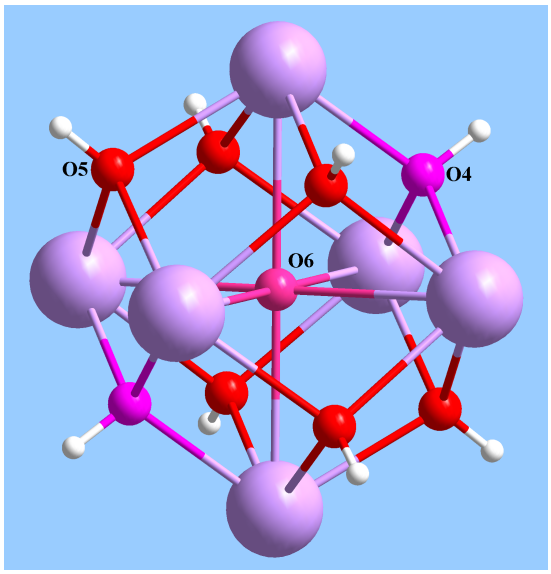

Figure S2. $[Er_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8]^{8+}$ cluster unit containing three different μ-O bridges, μ_3-O(O4): magenta; μ_3-O(O5): red; μ_6-O(O6): pink.

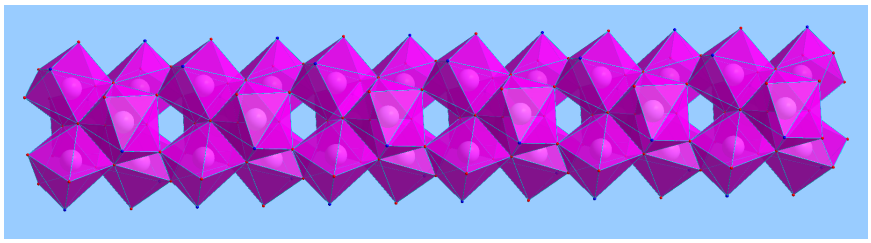

Figure S3. View of infinite 1D nano-sized Er-O-Er rods.

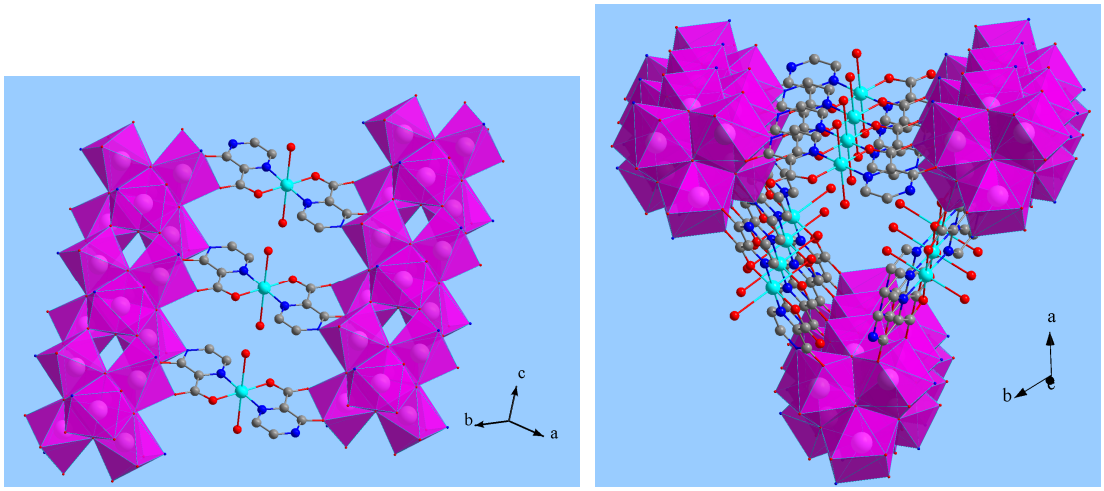

Figure S4. (left) View of two infinite 1D inorganic Er-O-Er rods linked by L^{Cu} SBUs; (right) Trigonal channel formed by L^{Cu} SBUs connecting with three offset 1D Er-O-Er rods.

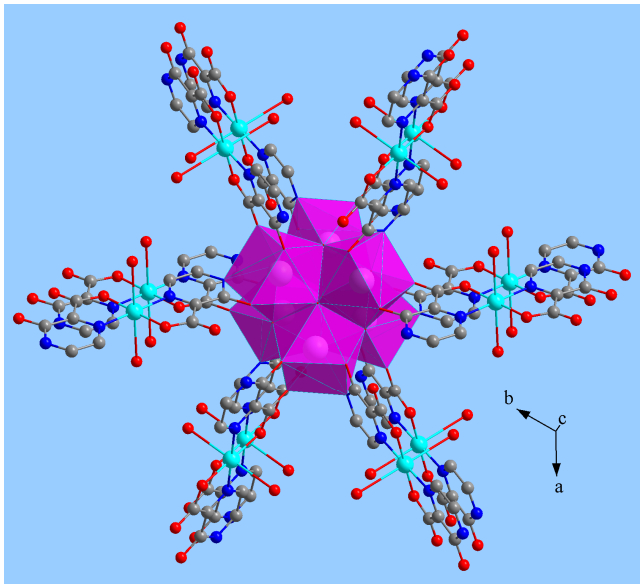

Figure S5. Each $[Er_6(\mu_6\text{-}O)(\mu_3\text{-}OH)_8]^{8+}$ cluster unit bridged by twelve L^{Cu} SBUs.

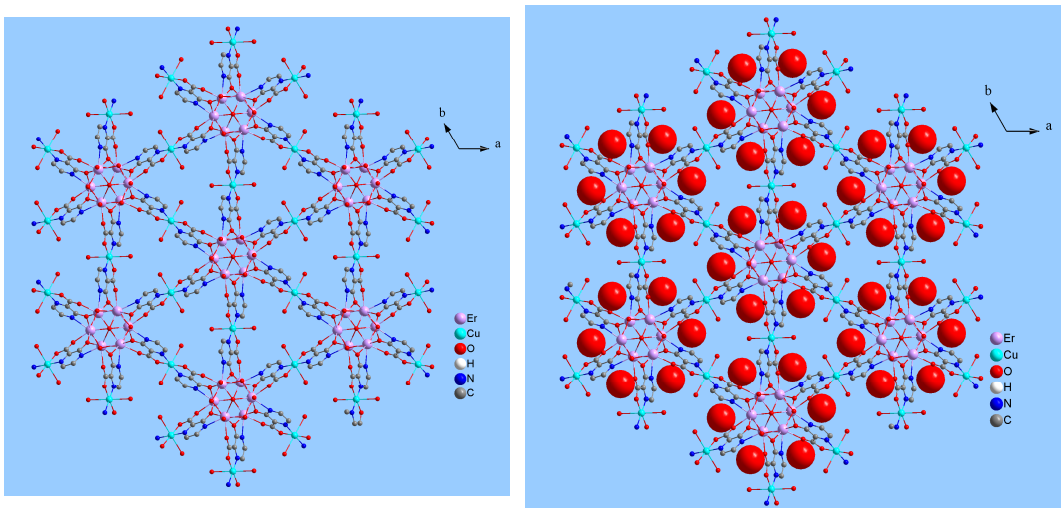

Figure S6. (left) View of each 1D nano-sized Er-O-Er rod linked by six equivalent ones to form the 3D network of **3** with trigonal channels along the *c*-axis direction; (right) View of the trigonal channels filling with the lattice water molecules.

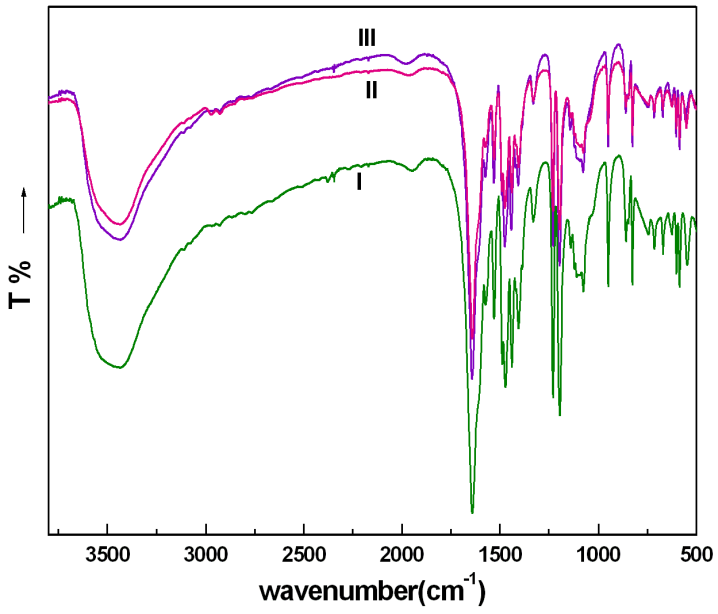

Figure S7. The IR spectra of **1-3. I (Dy)**; **II (Ho); III (Er)**

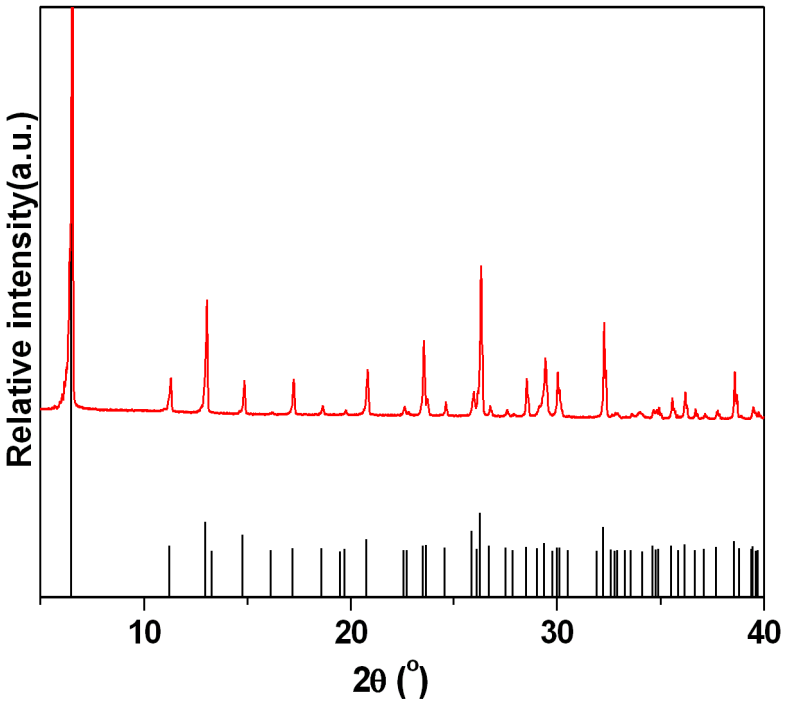

Figure S8 XPRD patterns for **3**: (top) measured at room temperature; (bottom) calculated on the basis of the structure determined by single-crystal X-ray diffraction.

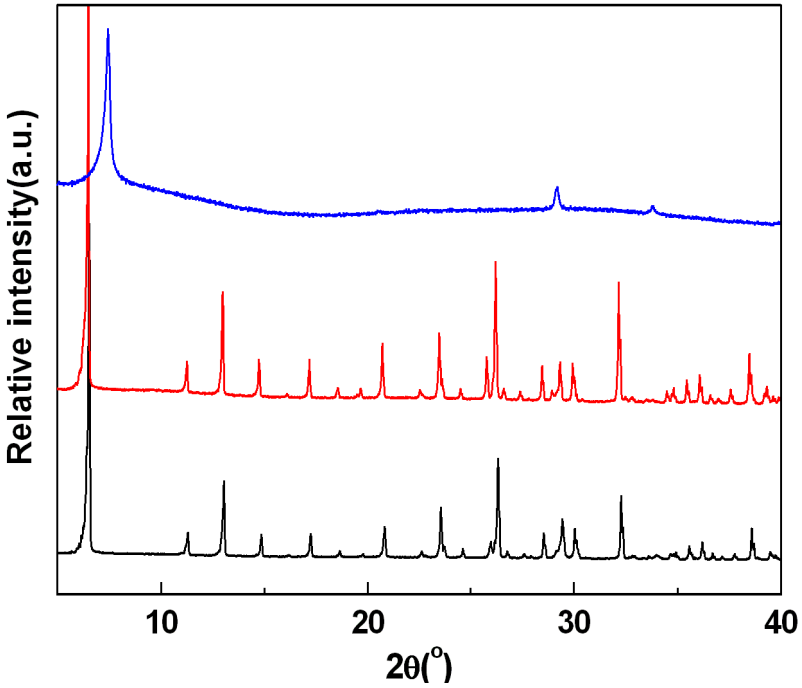

Figure S9 XPRD patterns of **3**: (black) measured at room temperature; (red) heated to 250 °C for 20min; (blue) heated to 360 °C for 20min under a nitrogen atmosphere. The diffraction peaks on 250 °C corresponded well to the pattern at room temperature in position, indicating the framework of **3** is stable before 250 ºC when the partly coordination water molecules were removed from the structure. However, the diffraction peaks on 360 ºC reveal the collapse of the whole framework.

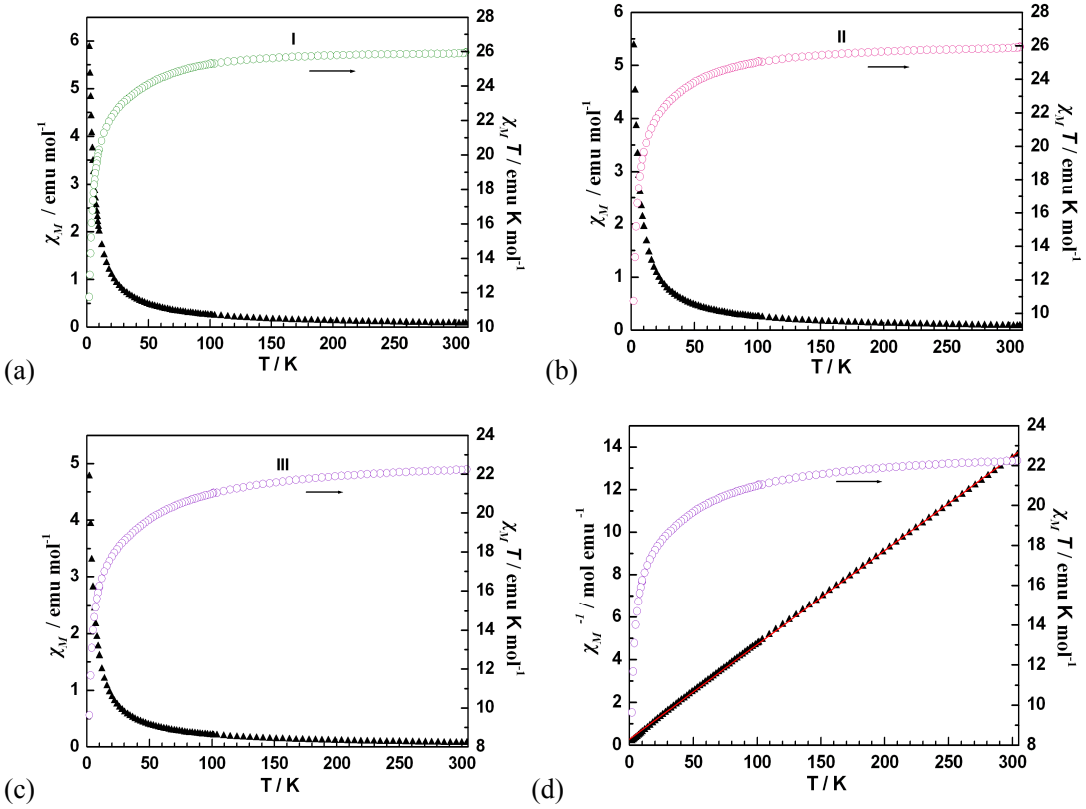

Figure S10. (a)(b)(c) Temperature dependence of χ_M and $\chi_M T$ for **1-3**, **I (Dy)**; **II (Ho); III (Er);** (d) Temperature dependence of $\chi_M T$ and χ_M^{-1} for **3**, the solid red line represents the best fit obtained from a Curie-Weiss law.

Table S1. Selected Bond Angles (o) for Compound **3**[a].

O4—Er1—O5	115.2(3)	O4—Er1—O1^{iii}	82.3(2)
O4—Er1—O5^{i}	74.96(14)	O5—Er1—O1^{iii}	139.16(11)
O5—Er1—O5^{i}	75.43(11)	O5^{i}—Er1—O1^{iii}	145.03(12)
O4—Er1—O1	85.9(2)	O1—Er1—O1^{iii}	70.95(5)
O5—Er1—O1	142.35(12)	O2—Er1—O1^{iii}	109.30(13)
O5^{i}—Er1—O1	81.14(13)	O5^{ii}—Er1—O1^{iii}	76.26(12)
O4—Er1—O2	150.63(12)	N1^{iii}—Er1—O1^{iii}	52.04(13)
O5—Er1—O2	74.19(13)	O4—Er1—O6	54.2(2)
O5^{i}—Er1—O2	81.31(14)	O5—Er1—O6	60.94(9)
O1—Er1—O2	73.45(13)	O5^{i}—Er1—O6	60.71(9)
O4—Er1—O5^{ii}	73.75(14)	O1—Er1—O6	129.19(9)
O5—Er1—O5^{ii}	74.28(11)	O2—Er1—O6	126.16(10)
O5^{i}—Er1—O5^{ii}	120.64(17)	O5^{ii}—Er1—O6	60.01(9)
O1—Er1—O5^{ii}	143.34(12)	N1^{iii}—Er1—O6	135.67(12)
O2—Er1—O5^{ii}	134.50(13)	O1^{iii}—Er1—O6	123.87(8)
O4—Er1—N1^{iii}	131.12(17)	O3^{iv}—Cu1—O3	180.0(5)
O5—Er1—N1^{iii}	94.52(14)	O3^{iv}—Cu1—N2	96.1(2)
O5^{i}—Er1—N1^{iii}	153.18(14)	O3—Cu1—N2	83.9(2)
O1—Er1—N1^{iii}	93.33(15)	O3^{iv}—Cu1—N2^{iv}	83.9(2)
O2—Er1—N1^{iii}	71.98(16)	O3—Cu1—N2^{iv}	96.1(2)
O5^{ii}—Er1—N1^{iii}	78.73(15)	N2—Cu1—N2^{iv}	180.0(4)
O3—Cu1—O2w^{v}	92.88(5)	N2—Cu1—O2w^{v}	87.21(6)
O3^{iv}—Cu1—O2w^{v}	87.12(5)	N2^{iv}—Cu1—O2w^{v}	92.80(6)
O2w^{v}—Cu1—O2w^{vi}	180.00(2)		

[a] Symmetry codes for **3**: (i) 1/3+x-y, -1/3+x, 2/3-z; (ii) 1/3+y, 2/3-x+y, 2/3-z; (iii) 1/3+y, 2/3-x+y, -1/3-z; (iv) 2-x, 1-y, -z; (v) 2-x, 1-y, 1-z; (vi) x, y, 1+z.