Polymeric double-anion templated Er_{48} nano-tubes

Mingyan Wu,[a] Feilong Jiang,[a] Daqiang Yuan,[a] Jiandong Pang,[ab] Jinjie Qian,[ab] Shaeel A. AL-Thabaiti[c] and Maochun Hong*[ac]

[a] State Key Laboratory of Structure Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, China.

[b] Graduate School of the Chinese Academy of Sciences, Beijing, 100049, China.

[c] Department of Chemistry, Faculty of Science, King Abdulaziz University, Jeddah, 21589, Saudi Arabia.

E-mail: hmc@fjirsm.ac.cn; Fax: +86-591-83794946; Tel: +86-591-83792460.

Supporting Information

Experimental Section

Figure S1 The 48-nuclaerity Er(III) cluster. Light green, Er; Red, oxygen; Blue, Nitrogen; Gray, Carbon.

Figure S2 (a) The wheel-like Er_{18} unit (b) The Er_{12} "Star of David". (c) The other six Er cations in six Er_4 uints respectively also form a perfect plane. The Er_{12} cations in "Star of David" is in green and the other six Er cations in six Er_4 uints respectively in blue.

Figure S3 The ring-like Er_{12} unit.

Figure S4 PXRD for complex **1**. The diffraction angle θ is from 3.5 to 45°.

Figure S5 For **1**, *M vs*. *H* data at 2K.

Experimental Section

Materials and methods

All reactants were reagent grade and used as purchased without further purification. Elemental analyses for C, H, N were carried out on a German Elementary Vario EL III instrument. The power X-ray diffraction (XRD) patterns were collected by a Rigaku DMAX2500 X-ray diffractometer using Cu Kα radiation (λ = 0.154 nm). Magnetic data were recorded on polycrystalline samples with Quantum Design PPSM-9T and MPMS-XL systems.

Synthesis

65mg (1.0 mmol) NaN_3 was added to the solution of 49 mg (0.4 mmol) nicotinic acid, 17 mg (0.2 mmol) $NaNO_3$ and 77 mg (0.2 mmol) $ErCl_3 \cdot 6H_2O$ in 6 mL H_2O. The Teflon-lined bomb was sealed and rasised at the temperature of 190 ℃ for three days. Cooling the bomb slowly at 1 ℃ / 10min afforded the expected colorless prism crystals **1**. Yield, c.a. 13 mg (19.11 %, based on Er). Anal. Calcd for complex **1**:calcd C, 19.36; H, 2.36; N,4.10; found C, 19.42; H, 2.36; N, 3.98.

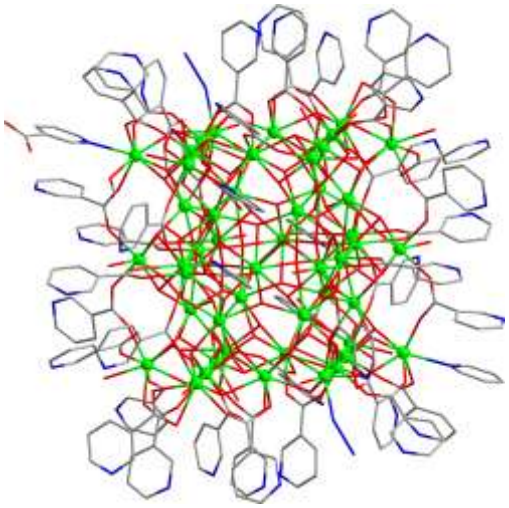
X-ray data collection and sructural determination

The data of complex **1** was collected on a Rigaku MM007 CCD diffractometer equipped with a graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 293 K. This structure was resolved by the direct method and refined by full-matrix least-squares fitting on F^2 by *SHELX*-97 software package.[1] All non-hydrogen atoms were refined with anisotropic thermal parameters except several solvent molecules. The hydrogen atoms of NA ligands are located into their theoretic positions and fixed by the riding mode. The hydrogen atoms which are in hydrogen bonding to the Cl^- and NO_3^- anions were located at geometrically calculated positions and refined by riding. More details on the crystallographic studies as well as atomic displacement parameters are given in Supporting Information as CIF files. Crystallographic data for the structures reported in this paper have been deposited in the Cambridge Crystallographic Data Center with CCDC reference number 959125 for complexes **1**.

Crystal and refinement details for complex 1

1, $C_{264}H_{384}N_{48}O_{240}Cl_8Er_{48}$, M = 16382.25, red crystals, 0.05 mm x 0.06 mm x 0.08 mm. Triclinic, space group P-1, a = 23.170(4) Å, b = 24.088(5) Å, c = 24.896(4) Å, α = 68.750(10) °, β = 66.393(10)°, γ = 62.015(8) °, V = 10979(4) $Å^3$, Z = 1. F(000) = 7624, $2\theta_{max}$ = 54.53°, 47359 reflections collected, 34096 unique (Rint = 0.0834). Final R1 = 0.0534, wR2 = 0.1291, $GooF$ = 0.983, R indices based on 34097 reflections with $I > 2\sigma(I)$ (refinement on F^2).

Electronic Supplementary Material (ESI) for Chemical Communications



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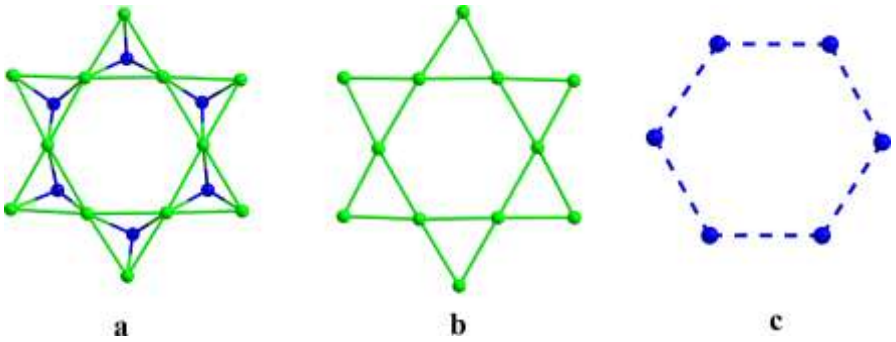

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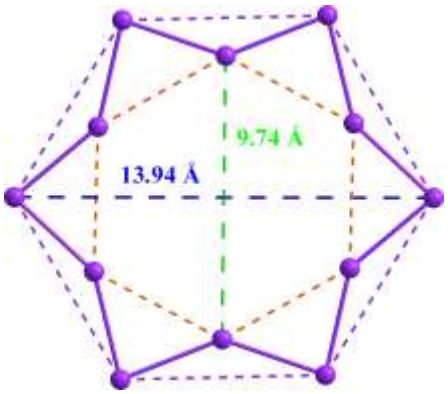

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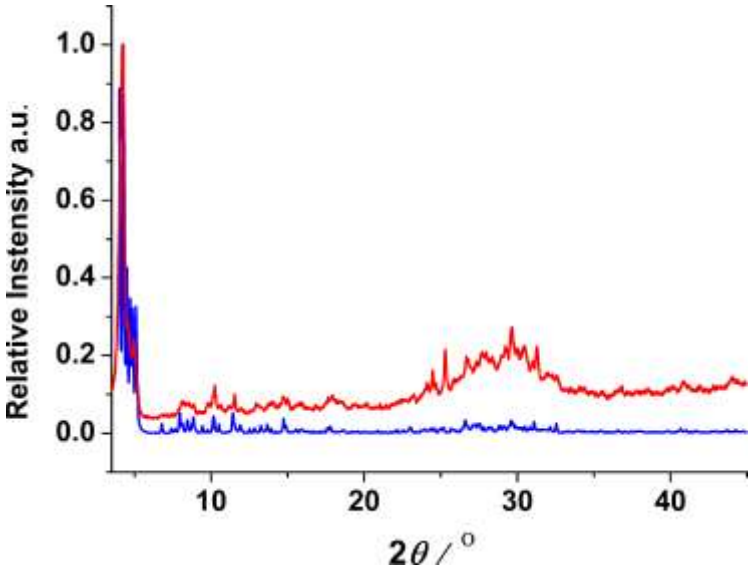

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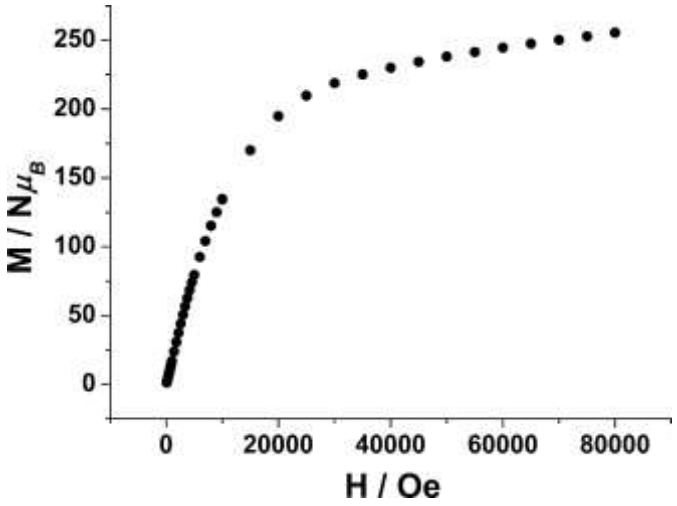

Figure S5 For **1**, *M vs*. *H* data at 2K.

Reference:

1. Sheldrick, G. M. *University of Göttingen: Germany*, **1997**.