Supporting Information

Isolation, Structure and Magnetic Property of Two Novel Core-Shell 3d-4f Hetermetallic Nanoscale Clusters

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Materials and Methods

All the chemicals purchased were of reagent grade and used without further purification. Elemental analyses (C, H and N) were performed on a Perkin-Elmer 2400 elemental analyzer. Na and Ni analyses are performed by ICP OPTMA20000V Plasma emission spectrometer, while the analysis for Cl is measured by Energy Dispersive Spectrometer (HITACHI S-4800 FESEM). Powder X-ray diffraction data were performed on a Bruker D8 Advance diffractometer with Cu Kα radiation (λ = 1.54056 Å), with a step speed of 0.1 ° per second.IR spectra of compound **1** were recorded with a Nicolet Impact 410 FTIR spectrometer with pressed KBr pellets from 4000 to 400 cm^{-1}. Single-crystal XRD data of **1** were obtained from a Bruker Apex II CCD with Mo-Kα radiation (λ = 0.71073 Å) at 296K. TG measurement was carried out on a Diamond thermogravimetric analyzer in flowing N_2 atmosphere from 17 to 1000 °C with a heating rate of 10 °C min^{-1}. The direct current magnetic data were measured at temperature between 1.8 and 300 K, and the magnetisation isothermal measurements were made in fields of between 0 and 7 T on MPMS-XL7 SQUID magnetometer.

Experimental Section

Synthesis of 1: A mixture of Nd_2O_3 (0.1668 g, 0.50 mmol), $Ni(OAc)_2{\cdot}4H_2O$ (0.1234 g,0.50 mmol), IDA (0.0628 g, 0.48 mmol), NaCl (0.0060 g, 0.10 mmol) in the mixture of distilled water (5 mL) and EtOH (10 mL) was stirred for 12 hours at room temperature. The pH of resulting solution was adjusted to 5.0 by the addition of 1 M HCl aqueous solution. This solution was then sealed in a 25 mL Teflon-lined stainless steel autoclave and heated under autogenous pressure at 180 °C for 8 days. After cooling to room temperature, blue square slice crystals were filtered off, washed with ethanol, and dried at room temperature for 24 h (Yield 46% based on Nd). Calcd.(%) C: 13.97; H: 2.00; N: 3.46; Na: 0.54; Cl: 1.25; Ni: 14.67; Found (%): C: 13.78; H: 1.90; N: 3.35; Na: 0.62; Cl: 1.31; Ni: 15.02 (Na and Ni analyses are performed by ICP OPTMA20000V Plasma emission spectrometer, while the analysis for Cl is measured by Energy Dispersive Spectrometer).

Synthesis of 2: Compound **2** was prepared in a procedure similar to that of **1**, except that Pr_4O_{11} (0.1663g, 0.16 mmol) was utilized instead of Nd_2O_3, blue square slice crystals were obtained. (Yield 61%

based on Pr). Calcd.(%) C:12.76; H: 2.13; N: 3.31; Na: 0.14; Cl: 2.09; Ni: 13.18; Found (%): C: 12.53; H: 2.27; N: 13.18; Na: 0.21; Cl: 2.00; Ni: 12.82.

Crystal data of **1** :$C_{194}H_{305}Cl_6N_{42}$ Na_2 Nd_{38} $Ni_{42.50}$ O_{345}, *Mr*=16980.78, orthorhombic, *Pnnm, a*=28.703(3), *b*=33.963(3), *c*=24.664(3) Å, *V*=24043(4) Å^3, Z=2, μ = 5.786 mm^{-1},ρ =2.346 g·cm^{-3}, *F* (000)=16234, θ_{max}=25.02°.104792 measured reflections, 21142 independent reflections. Based on these and 1603 parameters, R_1=0.0689 (I>2σ(I)), wR_2=0.2111 (all data) were obtained. GOF=1.018.

Crystal data of **2**:$C_{180}H_{377}Cl_{10}N_{40}NaPr_{42}Ni_{38}O_{331}$, *Mr*=16924.88, Monoclinic, $P2_1/n$, *a*=22.761(3), *b*=28.178(3), *c*=35.469(3) Å, *V*=22311(3) Å^3, Z=2, μ = 6.223 mm^{-1},ρ =2.521 g.cm^{-3}, *F* (000)=16236, θ_{max}=25.02°.127095 measured reflections, 38579 independent reflections. Based on these and 1524 parameters, R_1=0.0726 (I>2σ(I)), wR_2=0.208 (all data) were obtained. GOF=1.086. Crystal size (mm):0.14×0.13×0.12. CCDC 1504913 and 1504914 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre. Powder X-ray diffraction data were performed on a Bruker D8 Advance diffractometer with Cu Kα radiation (λ = 1.54056 Å), with a step speed of 0.1 ° per second. IR spectra of both compounds were recorded with a Nicolet Impact 410 FTIR spectrometer with pressed KBr pellets from 4000 to 400 cm^{-1}. Single-crystal XRD data of 1 were obtained from a Bruker Apex II CCD with Mo-Kα radiation (λ = 0.71073 Å) at 296K. TG measurement was carried out on a Diamond thermogravimetric analyzer in flowing N_2 atmosphere from 17 to 1000 °C with a heating rate of 10 °C min^{-1}. The direct current magnetic data were measured at temperature between 1.8 and 300 K, and the magnetisation isothermal measurements were made in fields of between 0 and 7 T on MPMS-XL7 SQUID magnetometer. Experimental susceptibilities were corrected for the diamagnetism estimated Pascal's tables and for sample holder by previous calibration.

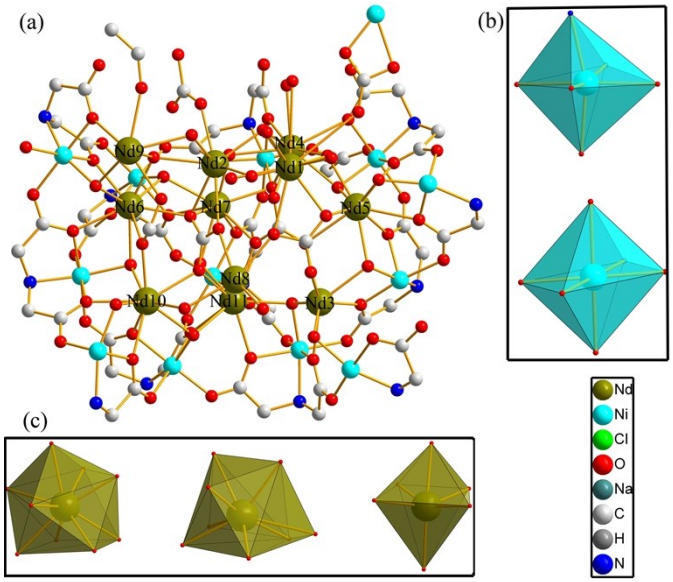


Fig.S1 (a) View of the petaloid asymmetric unit of complex **1.** (For clarity, hydrogen atoms, free Na^+ and Cl^- ions are omitted); (b) The coordination modes of Ni; (c) The coordination modes of Nd

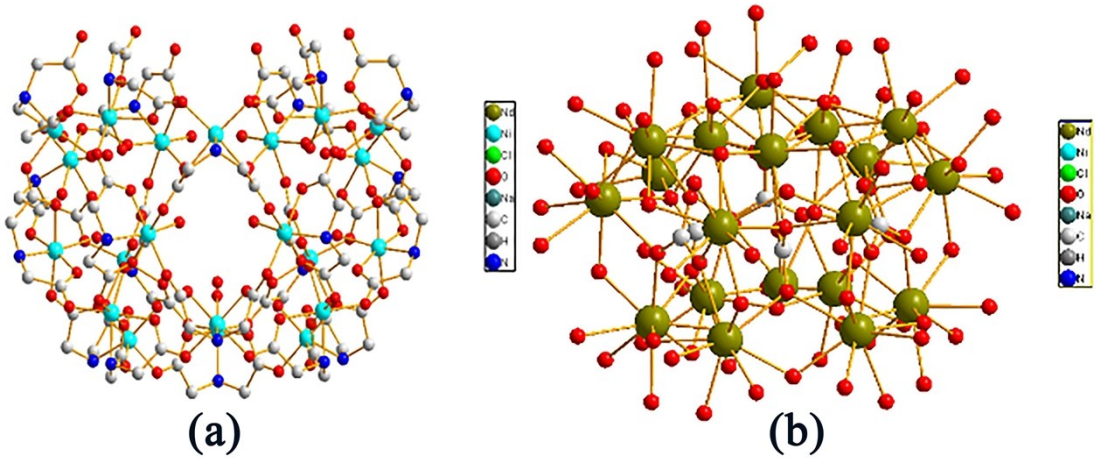


Fig.S2 (a) Ball-and-stick view of the metal shell {Ni_{21}} in compound **1**; (b) Ball-and-stick view of the metal core-shell {Nd19} in compound **1**.

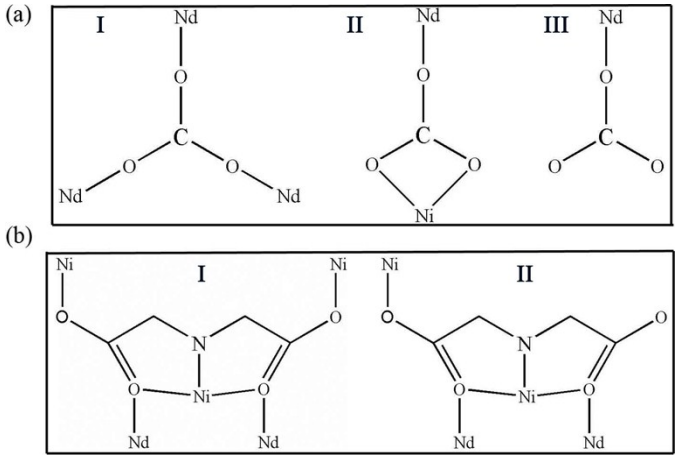


Fig.S3 The coordination modes of CO_3^{2-} and IDA ligands in **1**

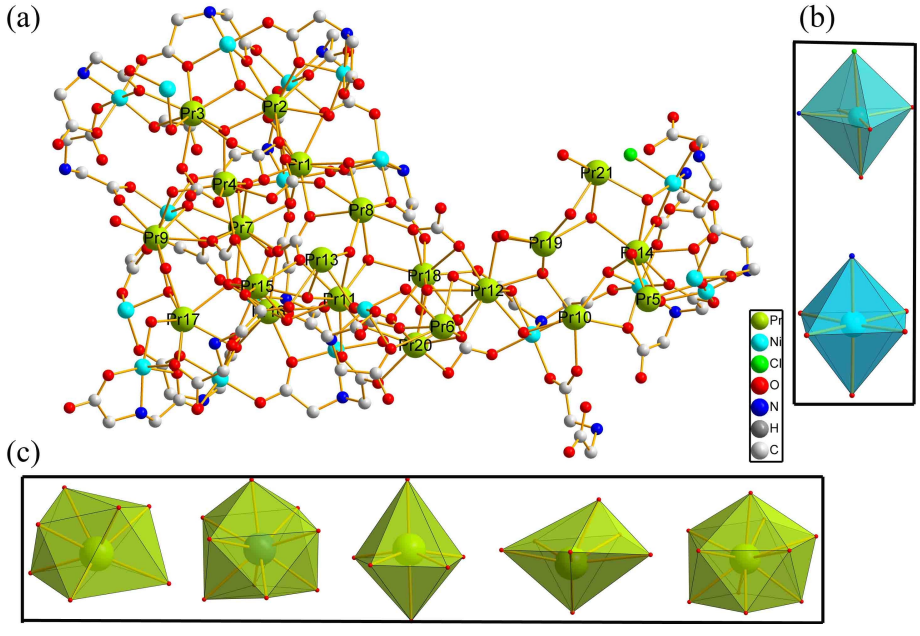


Fig.S4 (a) View of the petaloid asymmetric unit of compound **2**. (For clarity, hydrogen atoms, free ethanol molecules and Cl^- ions are omitted); (b) The coordination modes of Ni; (c) The coordination modes of Pr.

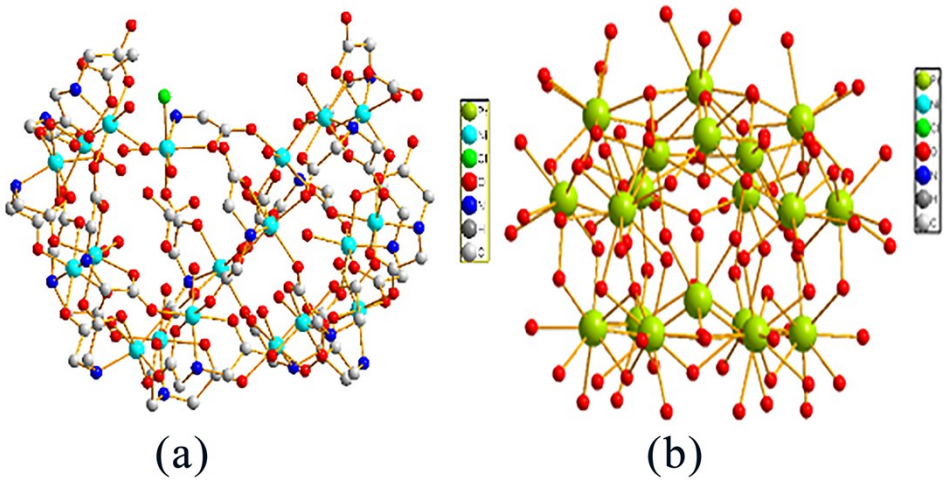


Fig.S5 (a) Ball-and-stick view of the metal shell $\{Ni_{19}\}$ in compound **2**; (b) Ball-and-stick view of the metal core-shell $\{Pr_{19}\}$ in compound **2**.

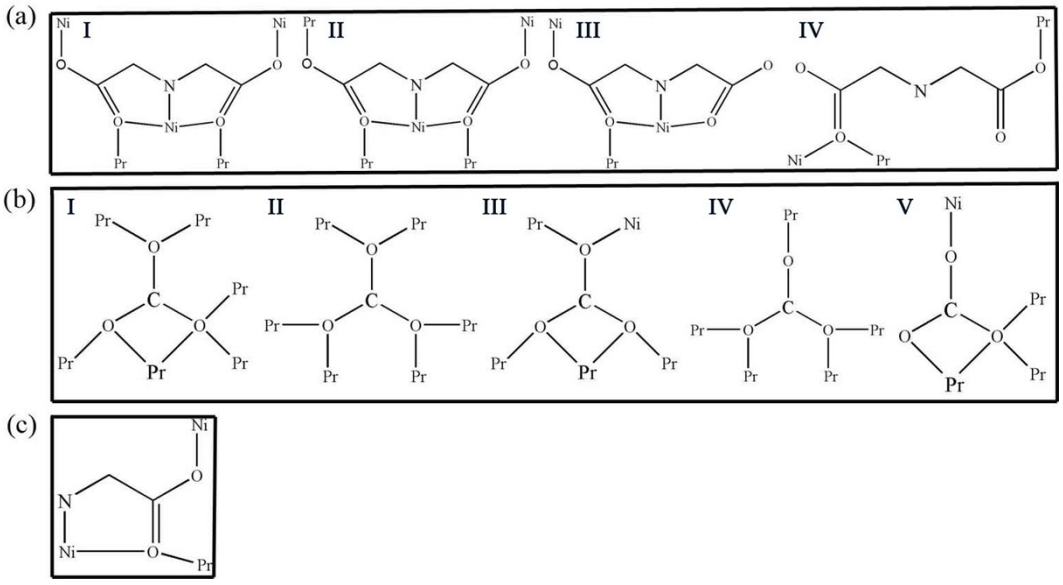


Fig.S6 The coordination modes of IDA, CO_3^{2-} and glycine ligands in **2**

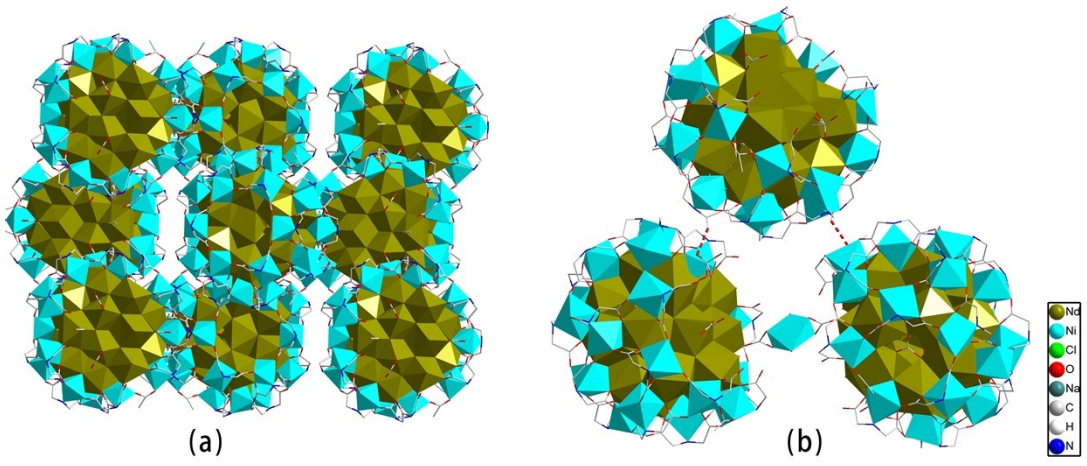


Fig. S7. (a) The 3D framwork of compound **1** along the b-axis; (b) hydrogen bonding interactions only (C–H···O) was indicated in compound **1**.

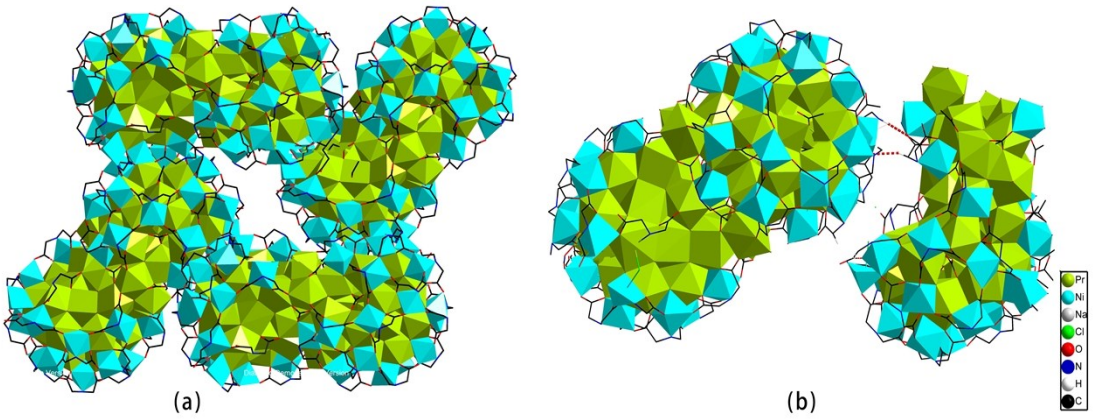


Fig. S8. (a) The 3D framwork of compound **2** along the c-axis; (b) hydrogen bonding interactions only (C–H···O) was indicated in compound **2**

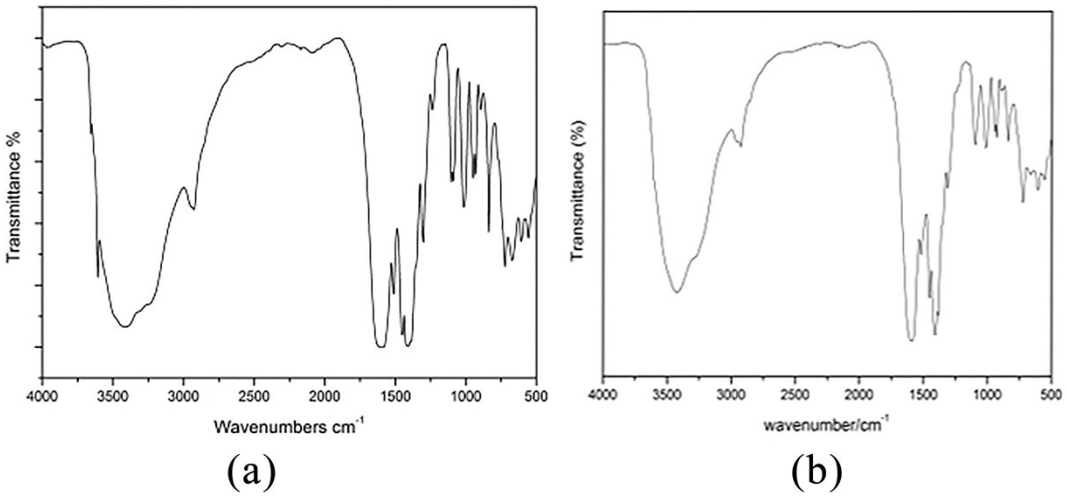


Fig.S9 The IR spectrum of compound **1** (a) and **2** (b).

The FTIR spectrum of compound **1** is shown in Fig.S9a. A strong peak at 3426 cm^{-1} can be attributed to the stretching vibration of O-H in ligand and aqua molecule. Two strong peaks at 1603 cm^{-1} and 1302 cm^{-1} are ascribed to carboxyl and OAc^- from IDA, three peaks from 1099cm^{-1} to 944cm^{-1} corresponds to ethanol molecule, absorptions from 554 cm^{-1} to 836 cm^{-1} are due to $\nu_{Nd\text{-}O}$ and $\nu_{Ni\text{-}N}$ vibrations.

The FTIR spectrum of compound **2** is shown in Fig. S9b. A strong peak at 3416 cm^{-1} can be attributed to the stretching vibration of O-H in ligand and aqua molecule. Two strong peaks at 1605 cm^{-1} and 1309 cm^{-1} are ascribed to carboxyl and OAc^- from IDA, three peaks from 1097cm^{-1} to 927cm^{-1}

corresponds to ethanol molecule, absorptions from 611 cm^{-1} to 839 cm^{-1} are due to $\nu_{Pr\text{-}O}$ and $\nu_{Ni\text{-}N}$ vibrations.

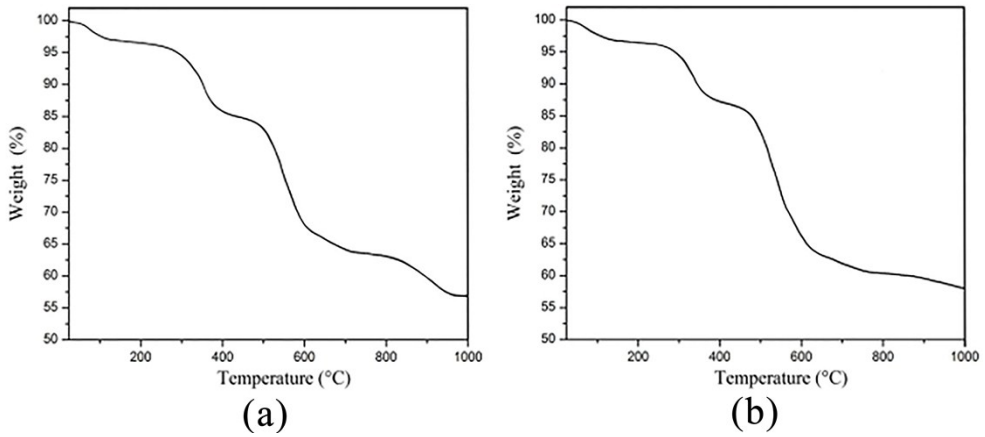
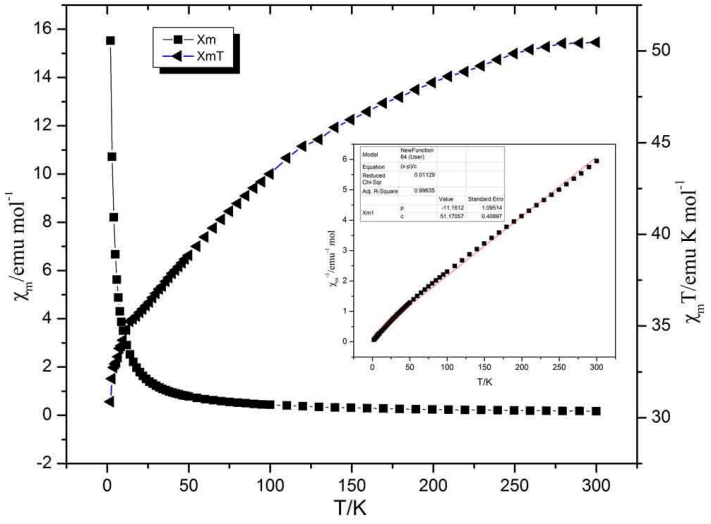


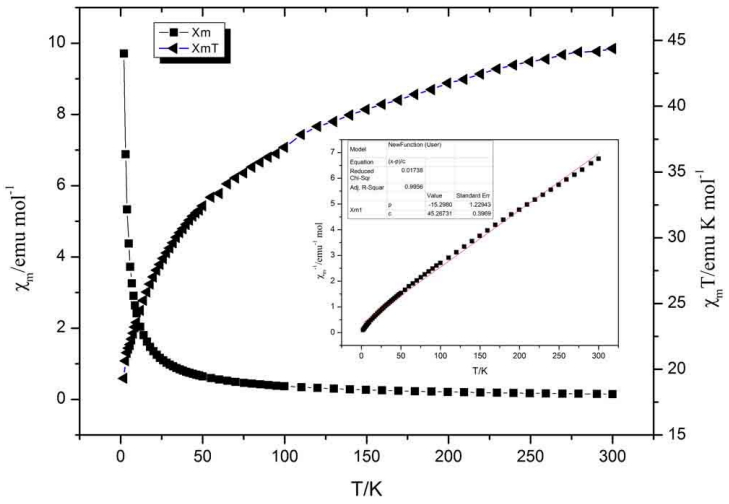
Fig S10. TG curve for compound **1**(a) and **2** (b).

As shown in Fig. S10a, the TGA curve of compound **1** in a temperature range of 25-1000 °C exhibits a three step weight loss process. A mass loss of 3.01% in a temperature range of 25—121 °C corresponds to the removal of lattice water (the calculated value is 2.88%). A mass loss of 4.45% in a temperature range of 121-280°C corresponds to the removal of coordinated water and ethanol molecules (the calculated value is 4.16%). The mass loss after 280 °C can be attributed to the decomposition of IDA ligands and the collapse of the framework.

Compound **2** (shown in Fig.S10b) exhibits a three step weight loss process. A mass loss of 4.19% in a temperature range of 25-120 °C corresponds to the removal of lattice water (the calculated value is 4.35%). A mass loss of 4.58% in a temperature range of 120—290°C corresponds to the removal of coordinated water and ethanol molecules (the calculated value is 4.99%). The mass loss after 280 °C can be attributed to the decomposition of IDA ligands and the collapse of the framework.

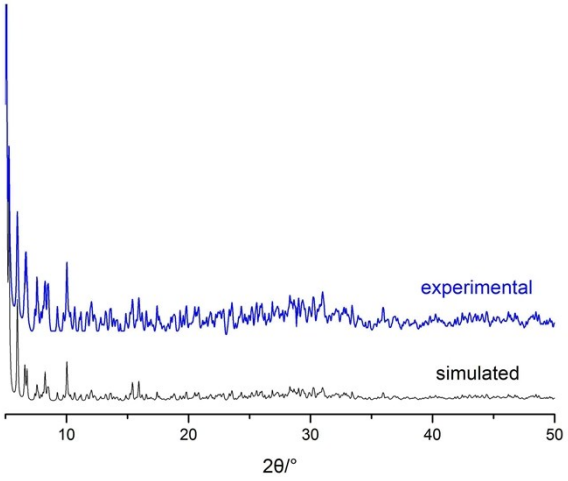


(a)

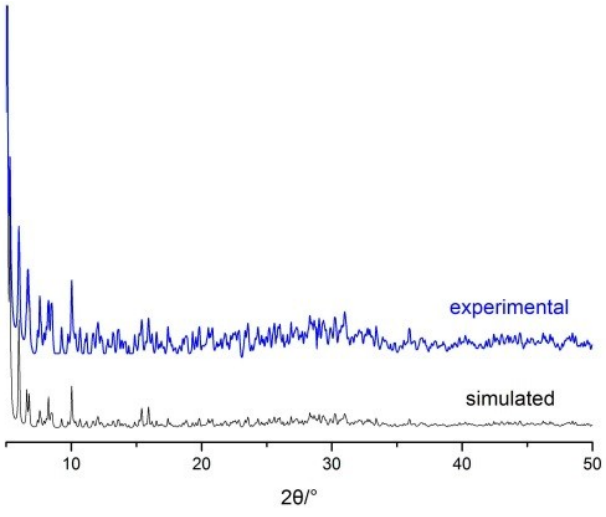


(b)

Fig.S11 Plots of T dependence of χ_m and χ_mT for**1** (a**)** and **2**(b)



(a)



(b)

Fig.S12. The experimental and simulated XRD patterns for **1** (a) and **2** (b)

Fig. S12 presents the powder X-ray diffraction patterns for the compounds **1** and **2**. Diffraction peaks of both the simulated and experimental patterns are well matched in relevant positions, showing the bulk products are purephases.

Table S1 The Crystallographic data of compound **1**.

Compound	**1**
Empirical formula	$C_{194}H_{305}Cl_6N_{42}\ Na_2\ Nd_{38}\ Ni_{42.50}\ O_{345}$
Formula weight	16980.78
Crystal system	Orthorhombic
Space group	*Pnnm*
a (Å)	28.703(3)
b (Å)	33.963(3)
c (Å)	24.664(3)
V (Å)	24043(4)
Z	2
D_c ($g{\cdot}cm^{-3}$)	2.346
μ (mm^{-1})	5.786
F (000)	16234
Crystal size (mm)	0.13×0.12×0.11
θ Range	0.93-25.02
Reflections collected	104792
Independent reflections	21142 [R_{int} = 0.2260]
Reflections observed [$I>2\sigma(I)$]	10964
Data/restraints/parameters	21142/419/1603
Goodness-of-fit on F^2	1.018
R/wR [$I>2\sigma(I)$]	0.0690/0.1728
R/wR (all data)	0.1634/0.2113
Max., Min. $\Delta\rho$ ($e{\cdot}Å^3$)	2.963, -3.785

Table S2 Selected bond distances (Å) for compound **1**

Bond lengths			
Nd(1)-O(1)	2.376(16)	Nd(11)-O(16)	2.409(8)
Nd(1)-O(5)	2.396(8)	Nd(11)-O(24)	2.448(8)
Nd(1)-O(5)#1	2.396(8)	Nd(11)-O(28)	2.451(7)
Nd(1)-O(17)#1	2.400(9)	Nd(11)-O(22)#1	2.490(8)
Nd(1)-O(17)	2.400(9)	Nd(11)-O(40)	2.492(9)
Nd(1)-O(5W)	2.46(2)	Nd(11)-O(35)	2.519(8)
Nd(1)-O(85)	2.69(2)	Nd(11)-O(15)	2.520(8)
Nd(1A)-O(1A)	2.427(14)	Nd(11)-O(44)	2.532(7)
Nd(1A)-O(72)	2.460(17)	Nd(11)-O(56)	2.571(8)
Nd(1A)-O(5)	2.569(8)	Ni(12)-O(54)	1.988(11)

Nd(1A)-O(5)#1	2.569(8)	Ni(12)-O(70)#1	2.054(8)
Nd(1A)-O(17)	2.610(9)	Ni(12)-O(70)	2.054(8)
Nd(1A)-O(17)#1	2.610(9)	Ni(12)-O(46)	2.062(8)
Nd(1A)-O(66)	2.797(15)	Ni(12)-O(46)#1	2.062(8)
Nd(2)-O(17)	2.380(9)	Ni(12)-N(10)	2.069(13)
Nd(2)-O(55)	2.396(8)	Ni(13)-O(15)	2.003(8)
Nd(2)-O(1)	2.405(10)	Ni(13)-O(63)	2.030(8)
Nd(2)-O(83)	2.473(11)	Ni(13)-O(19)	2.052(8)
Nd(2)-O(33)	2.517(9)	Ni(13)-O(56)	2.072(8)
Nd(2)-O(2)	2.586(14)	Ni(13)-O(27)	2.073(8)
Nd(2)-O(13)	2.654(9)	Ni(13)-N(7)	2.076(11)
Nd(2)-O(75)	2.682(10)	Ni(14)-O(34)	2.008(11)
Nd(2)-O(73)	2.947(8)	Ni(14)-O(6)#1	2.059(8)
Nd(2A)-O(33)	2.187(9)	Ni(14)-O(6)	2.059(8)
Nd(2A)-O(83)	2.227(9)	Ni(14)-O(30)	2.072(8)
Nd(2A)-O(1A)	2.392(19)	Ni(14)-O(30)#1	2.072(8)
Nd(2A)-O(55)	2.413(9)	Ni(14)-N(9)	2.117(14)
Nd(2A)-O(17)	2.436(9)	Ni(15)-O(16)	2.020(7)
Nd(2A)-O(2A)	2.439(14)	Ni(15)-O(51)	2.035(8)
Nd(2A)-O(13)	2.929(9)	Ni(15)-O(36)	2.052(8)
Nd(3)-O(16)	2.426(8)	Ni(15)-O(62)	2.074(8)
Nd(3)-O(25)	2.453(8)	Ni(15)-N(4)	2.099(9)
Nd(3)-O(47)	2.468(6)	Ni(15)-O(28)	2.107(8)
Nd(3)-O(62)	2.503(8)	Ni(16)-O(60)	2.019(9)
Nd(3)-O(22)#1	2.503(8)	Ni(16)-O(11)	2.026(8)
Nd(3)-O(54)	2.506(6)	Ni(16)-O(32)	2.036(8)
Nd(3)-O(12)	2.518(7)	Ni(16)-O(18)	2.091(8)
Nd(3)-O(53)	2.522(8)	Ni(16)-O(39)	2.092(8)
Nd(3)-O(70)#1	2.549(8)	Ni(16)-N(1)	2.114(11)
Nd(4)-O(73)	2.437(8)	Ni(17)-O(53)	2.005(8)
Nd(4)-O(23)	2.483(8)	Ni(17)-O(7)	2.061(8)
Nd(4)-O(45)	2.510(8)	Ni(17)-O(43)	2.061(8)
Nd(4)-O(5)	2.513(8)	Ni(17)-O(42)#1	2.064(9)
Nd(4)-O(55)	2.520(9)	Ni(17)-O(25)	2.067(8)
Nd(4)-O(17)	2.566(9)	Ni(17)-N(6)	2.084(10)
Nd(4)-O(71)	2.587(9)	Ni(18)-O(58)	1.978(8)
Nd(4)-O(77)	2.599(10)	Ni(18)-O(26)	2.041(8)
Nd(4)-O(8)	2.637(8)	Ni(18)-O(49)	2.047(8)
Nd(5)-O(5)	2.407(8)	Ni(18)-O(38)	2.084(8)
Nd(5)-O(45)	2.451(8)	Ni(18)-N(11)	2.086(11)
Nd(5)-O(25)	2.463(8)	Ni(18)-O(21)	2.097(8)
Nd(5)-O(41)	2.466(8)	Ni(19)-O(4)	2.032(11)
Nd(5)-O(72)	2.519(7)	Ni(19)-O(31)#1	2.035(9)
Nd(5)-O(34)	2.532(6)	Ni(19)-O(31)	2.035(9)

Nd(5)-O(7)	2.559(8)	Ni(19)-O(29)	2.072(8)
Nd(5)-O(12)	2.631(8)	Ni(19)-O(29)#1	2.072(8)
Nd(5)-O(6)	2.643(8)	Ni(19)-N(12)	2.101(14)
Nd(6)-O(33)	2.415(8)	Ni(20)-O(48)	2.024(9)
Nd(6)-O(20)	2.453(9)	Ni(20)-O(52)	2.031(9)
Nd(6)-O(14)	2.464(7)	Ni(20)-O(35)	2.032(8)
Nd(6)-O(39)	2.505(7)	Ni(20)-O(37)	2.051(9)
Nd(6)-O(13)	2.509(8)	Ni(20)-N(2)	2.099(11)
Nd(6)-O(32)	2.526(8)	Ni(20)-O(24)	2.101(8)
Nd(6)-O(58)	2.541(8)	Ni(21)-O(67)	1.943(18)
Nd(6)-O(50)	2.604(8)	Ni(21)-O(23)	2.036(8)
Nd(6)-O(26)	2.620(9)	Ni(21)-N(8)	2.044(11)
Nd(7)-O(23)	2.409(8)	Ni(21)-O(77)	2.054(10)
Nd(7)-O(55)	2.440(8)	Ni(21)-O(68)	2.067(8)
Nd(7)-O(68)	2.446(8)	Ni(21)-O(61)	2.078(9)
Nd(7)-O(24)	2.465(7)	Ni(22)-O(79)	1.956(14)
Nd(7)-O(58)	2.495(8)	Ni(22)-O(8)	2.057(8)
Nd(7)-O(48)	2.517(9)	Ni(22)-O(59)	2.056(9)
Nd(7)-O(13)	2.557(8)	Ni(22)-O(45)	2.060(8)
Nd(7)-O(49)	2.628(8)	Ni(22)-N(3)	2.097(11)
Nd(7)-O(44)	2.632(7)	Ni(22)-O(41)	2.106(8)
Nd(8)-O(10)	2.367(12)	Ni(23)-O(69)	2.048(10)
Nd(8)-O(22)#1	2.375(8)	Ni(23)-O(20)	2.050(8)
Nd(8)-O(22)	2.375(8)	Ni(23)-O(14)	2.051(8)
Nd(8)-O(66)	2.412(16)	Ni(23)-O(57)	2.095(9)
Nd(8)-O(75)	2.504(10)	Ni(23)-N(5)	2.107(11)
Nd(8)-O(75)#1	2.504(10)	Ni(23)-O(1W)	2.116(16)
Nd(8)-O(40)#1	2.888(9)	Ni(24)-O(84)#2	2.01(3)
Nd(8)-O(40)	2.888(9)	Ni(24)-O(84)	2.01(3)
Nd(9)-O(74)	2.358(16)	Ni(24)-O(8W)#2	2.03(4)
Nd(9)-O(20)	2.444(8)	Ni(24)-O(8W)	2.03(4)
Nd(9)-O(20)#1	2.444(8)	Ni(24)-O(86)	2.28(3)
Nd(9)-O(33)	2.529(8)	Ni(24)-O(86)#2	2.28(3)
Nd(9)-O(33)#1	2.529(8)	O(1)-Nd(2)#1	2.405(10)
Nd(9)-O(69)#1	2.611(10)	O(1A)-Nd(2A)#1	2.391(19)
Nd(9)-O(69)	2.611(10)	O(4)-Nd(10)#1	2.413(6)
Nd(9)-O(3)	2.619(11)	O(10)-Nd(10)#1	2.499(7)
Nd(9)-O(83)	2.64(2)	O(22)-Nd(11)#1	2.490(8)
Nd(10)-O(4)	2.413(6)	O(22)-Nd(3)#1	2.503(8)
Nd(10)-O(39)	2.441(8)	O(34)-Nd(5)#1	2.532(6)
Nd(10)-O(50)	2.485(8)	O(42)-Ni(17)#1	2.064(8)
Nd(10)-O(29)	2.493(7)	O(47)-Nd(3)#1	2.468(6)
Nd(10)-O(11)	2.496(8)	O(54)-Nd(3)#1	2.506(6)
Nd(10)-O(10)	2.498(7)	O(70)-Nd(3)#1	2.548(8)

Nd(10)-O(15)	2.500(8)	O(72)-Nd(5)#1	2.519(7)
Nd(10)-O(40)	2.527(9)	O(83)-Nd(2A)#1	2.227(9)
Nd(10)-O(27)	2.584(8)	O(83)-Nd(2)#1	2.473(11)

Table S3 Selected bond angles (°) for compound **1**O(1)-Nd(1)-

O(5)#1	105.7(3)	O(54)-Ni(12)-O(70)#1	84.2(3)
O(1)-Nd(1)-O(5)	105.7(3)	O(54)-Ni(12)-O(70)	84.2(3)
O(5)#1-Nd(1)-O(5)	109.2(4)	O(70)#1-Ni(12)-O(70)	83.9(5)
O(1)-Nd(1)-O(17)	68.8(3)	O(54)-Ni(12)-O(46)	98.5(3)
O(5)#1-Nd(1)-O(17)	174.4(3)	O(70)#1-Ni(12)-O(46)	92.5(3)
O(5)-Nd(1)-O(17)	72.3(3)	O(70)-Ni(12)-O(46)	175.3(3)
O(1)-Nd(1)-O(17)#1	68.8(3)	O(54)-Ni(12)-O(46)#1	98.5(3)
O(5)#1-Nd(1)-O(17)#1	72.3(3)	O(70)#1-Ni(12)-O(46)#1	175.3(3)
O(5)-Nd(1)-O(17)#1	174.4(3)	O(70)-Ni(12)-O(46)#1	92.5(3)
O(17)-Nd(1)-O(17)#1	105.6(4)	O(46)-Ni(12)-O(46)#1	91.0(5)
O(1)-Nd(1)-O(5W)	120.1(6)	O(54)-Ni(12)-N(10)	162.5(4)
O(5)#1-Nd(1)-O(5W)	107.9(3)	O(70)#1-Ni(12)-N(10)	82.8(3)
O(5)-Nd(1)-O(5W)	107.9(3)	O(70)-Ni(12)-N(10)	82.8(3)
O(17)-Nd(1)-O(5W)	76.2(3)	O(46)-Ni(12)-N(10)	93.8(3)
O(17)#1-Nd(1)-O(5W)	76.2(3)	O(46)#1-Ni(12)-N(10)	93.8(3)
O(1)-Nd(1)-O(85)	170.4(4)	O(15)-Ni(13)-O(63)	97.5(3)
O(5)#1-Nd(1)-O(85)	69.4(2)	O(15)-Ni(13)-O(19)	99.1(3)
O(5)-Nd(1)-O(85)	69.4(2)	O(63)-Ni(13)-O(19)	92.1(3)
O(17)-Nd(1)-O(85)	115.9(2)	O(15)-Ni(13)-O(56)	83.7(3)
O(17)#1-Nd(1)-O(85)	115.9(2)	O(63)-Ni(13)-O(56)	91.4(3)
O(5W)-Nd(1)-O(85)	69.5(7)	O(19)-Ni(13)-O(56)	175.2(3)
O(1A)-Nd(1A)-O(72)	116.0(9)	O(16)-Ni(15)-O(28)	84.7(3)
O(1A)-Nd(1A)-O(5)	130.4(2)	O(51)-Ni(15)-O(28)	94.1(3)
O(72)-Nd(1A)-O(5)	75.8(3)	O(36)-Ni(15)-O(28)	178.3(3)
O(1A)-Nd(1A)-O(5)#1	130.4(2)	O(62)-Ni(15)-O(28)	86.6(3)
O(72)-Nd(1A)-O(5)#1	75.8(3)	N(4)-Ni(15)-O(28)	81.7(3)
O(5)-Nd(1A)-O(5)#1	99.0(4)	O(53)-Ni(17)-O(42)#1	87.7(3)
O(1A)-Nd(1A)-O(17)	73.9(6)	O(7)-Ni(17)-O(42)#1	173.9(4)
O(72)-Nd(1A)-O(17)	132.9(2)	O(43)-Ni(17)-O(42)#1	86.4(4)
O(5)-Nd(1A)-O(17)	66.2(3)	O(53)-Ni(17)-O(25)	83.9(3)
O(5)#1-Nd(1A)-O(17)	135.3(3)	O(7)-Ni(17)-O(25)	82.7(3)
O(1A)-Nd(1A)-O(17)#1	73.9(6)	O(43)-Ni(17)-O(25)	101.7(3)
O(72)-Nd(1A)-O(17)#1	132.9(2)	O(42)#1-Ni(17)-O(25)	100.1(3)
O(5)-Nd(1A)-O(17)#1	135.3(3)	O(53)-Ni(17)-N(6)	83.1(3)
O(5)#1-Nd(1A)-O(17)#1	66.2(3)	O(7)-Ni(17)-N(6)	81.3(3)
O(17)-Nd(1A)-O(17)#1	94.2(4)	O(43)-Ni(17)-N(6)	93.1(3)
O(1A)-Nd(1A)-O(66)	65.8(9)	O(42)#1-Ni(17)-N(6)	97.4(3)
O(72)-Nd(1A)-O(66)	50.2(4)	O(25)-Ni(17)-N(6)	157.7(3)

O(5)-Nd(1A)-O(66)	107.7(3)	O(58)-Ni(18)-O(26)	84.5(3)
O(5)#1-Nd(1A)-O(66)	107.7(3)	O(58)-Ni(18)-O(49)	83.6(3)
O(17)-Nd(1A)-O(66)	116.9(3)	O(26)-Ni(18)-O(49)	85.3(3)
O(17)#1-Nd(1A)-O(66)	116.9(3)	O(58)-Ni(18)-O(38)	96.2(3)
O(17)-Nd(2)-O(55)	71.7(3)	O(31)-Ni(19)-O(29)	94.4(3)
O(17)-Nd(2)-O(1)	68.7(4)	O(31)#1-Ni(19)-O(29)	179.1(3)
O(55)-Nd(2)-O(1)	127.5(4)	O(4)-Ni(19)-O(29)#1	84.8(3)
O(17)-Nd(2)-O(83)	93.5(5)	O(31)-Ni(19)-O(29)#1	179.1(3)
O(55)-Nd(2)-O(83)	141.1(4)	O(31)#1-Ni(19)-O(29)#1	94.4(3)
O(1)-Nd(2)-O(83)	74.6(5)	O(29)-Ni(19)-O(29)#1	86.5(4)
O(17)-Nd(2)-O(33)	137.9(3)	O(4)-Ni(19)-N(12)	161.1(4)
O(55)-Nd(2)-O(33)	97.3(3)	O(31)-Ni(19)-N(12)	98.5(3)
O(1)-Nd(2)-O(33)	135.2(4)	O(31)#1-Ni(19)-N(12)	98.5(3)
O(83)-Nd(2)-O(33)	69.5(5)	O(29)-Ni(19)-N(12)	81.5(3)
O(17)-Nd(2)-O(2)	68.4(4)	O(29)#1-Ni(19)-N(12)	81.5(3)
O(55)-Nd(2)-O(2)	70.9(4)	O(71)-Nd(4)-O(8)	68.7(3)
O(1)-Nd(2)-O(2)	121.4(5)	O(77)-Nd(4)-O(8)	88.8(3)
O(17)-Nd(4)-O(71)	65.0(3)	O(16)-Nd(3)-O(25)	119.7(3)
O(73)-Nd(4)-O(77)	132.9(3)	O(16)-Nd(3)-O(47)	134.5(3)
O(23)-Nd(4)-O(77)	67.1(3)	O(25)-Nd(3)-O(47)	73.7(4)
O(45)-Nd(4)-O(77)	114.9(3)	O(16)-Nd(3)-O(62)	67.9(3)
O(5)-Nd(4)-O(77)	156.0(3)	O(25)-Nd(3)-O(62)	133.1(3)
O(55)-Nd(4)-O(77)	71.1(3)	O(47)-Nd(3)-O(62)	137.4(3)
O(17)-Nd(4)-O(77)	113.4(3)	O(16)-Nd(3)-O(22)#1	70.9(3)
O(71)-Nd(4)-O(77)	67.9(3)	O(25)-Nd(3)-O(22)#1	144.3(3)
O(73)-Nd(4)-O(8)	134.0(3)	O(47)-Nd(3)-O(22)#1	76.3(4)
O(23)-Nd(4)-O(8)	116.1(3)	O(62)-Nd(3)-O(22)#1	82.5(3)
O(45)-Nd(4)-O(8)	65.6(3)	O(16)-Nd(3)-O(54)	131.8(3)
O(5)-Nd(4)-O(8)	70.1(3)	O(25)-Nd(3)-O(54)	108.0(3)
O(55)-Nd(4)-O(8)	156.8(3)	O(47)-Nd(3)-O(54)	63.8(3)
O(17)-Nd(4)-O(8)	113.6(3)	O(62)-Nd(3)-O(54)	75.2(3)
O(16)-Nd(3)-O(70)#1	124.2(3)	O(22)#1-Nd(3)-O(54)	74.7(3)
O(25)-Nd(3)-O(70)#1	70.6(3)	O(16)-Nd(3)-O(12)	73.2(2)
O(47)-Nd(3)-O(70)#1	101.3(3)	O(25)-Nd(3)-O(12)	70.0(3)
O(62)-Nd(3)-O(70)#1	69.2(3)	O(47)-Nd(3)-O(12)	72.1(3)
O(22)#1-Nd(3)-O(70)#1	135.0(3)	O(62)-Nd(3)-O(12)	141.1(3)
O(54)-Nd(3)-O(70)#1	64.9(3)	O(22)#1-Nd(3)-O(12)	82.7(2)
O(12)-Nd(3)-O(70)#1	140.4(3)	O(54)-Nd(3)-O(12)	133.8(3)
O(53)-Nd(3)-O(70)#1	68.0(3)	O(16)-Nd(3)-O(53)	68.8(3)
O(73)-Nd(4)-O(23)	74.9(3)	O(25)-Nd(3)-O(53)	66.3(3)
O(73)-Nd(4)-O(45)	77.4(3)	O(47)-Nd(3)-O(53)	140.0(4)
O(23)-Nd(4)-O(45)	73.0(3)	O(62)-Nd(3)-O(53)	76.9(3)
O(73)-Nd(4)-O(5)	71.0(3)	O(22)#1-Nd(3)-O(53)	139.1(3)
O(23)-Nd(4)-O(5)	132.0(3)	O(54)-Nd(3)-O(53)	131.2(3)

O(45)-Nd(4)-O(5)	67.4(3)	O(12)-Nd(3)-O(53)	91.7(2)
O(73)-Nd(4)-O(55)	69.1(3)	O(23)-Nd(4)-O(55)	67.3(3)

Table S4 Hydrogen bond interactions in compound **1**

D—H···A	d(D···H) /Å	d(H···A)/ Å	d(D···A)/Å	D—H···A (°)
C1-H1A··O79	0.97	2.49	3.151(18)	125
C14-H14A··O64	0.97	2.46	3.36(2)	153
C14-H14B··O21	0.97	2.41	3.144(15)	132
C15-H15A··O21	0.97	2.39	3.149(15)	134
C15-H15B··O38	0.97	2.53	3.054(14)	114
C20-H20A··O36	0.97	2.48	3.415(17)	161
C204-H20D··O9	0.96	1.81	2.430(16)	119
C30-H30A··O63	0.97	2.45	3.361(16)	156
C33-H33A··O13W	0.97	2.48	3.270(18)	138

Table S5 The Crystallographic data of compound **2**.

Compound	**2**
Empirical formula	$C_{180}H_{382}Cl_{10}N_{40}Ni_{38}Pr_{42}O_{333}$
Formula weight	16938.93
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	22.761(2)
b (Å)	28.178(2)
c (Å)	35.469(3)
V (Å)	22311(3)
Z	2
D_c (g·cm^{-3})	2.521
μ (mm^{-1})	6.223
F (000)	16236
Crystal size (mm)	0.14×0.13×0.12
θ Range	0.93-25.02
Reflections collected	127095
Independent reflections	38579 [R_{int} = 0.2260]
Reflections observed [$I>2\sigma(I)$]	23130
Data/restraints/parameters	38579/19/1524
Goodness-of-fit on F^2	1.086

R/wR [$I>2\sigma(I)$]	0. 0727/0.1812
R/wR (all data)	0.1392/0.2082
Max., Min. $\Delta\rho$ (e·Å^3)	4.067, -2.244

Table S6 Selected bond distances (Å) for compound **2**

Bond distances			
Pr(1)-O(14)	2.443(8)	Pr(14)-O(4)#1	2.559(7)
Pr(1)-O(24)	2.445(8)	Pr(14)-O(22)	2.560(8)
Pr(1)-O(11)	2.460(8)	Pr(14)-O(118)	2.581(9)
Pr(1)-O(15)	2.491(8)	Pr(14)-O(91)	2.596(9)
Pr(1)-O(45)	2.507(8)	Pr(15)-O(12)#1	2.400(7)
Pr(1)-O(79)	2.522(8)	Pr(15)-O(50)	2.425(8)
Pr(1)-O(95)	2.564(8)	Pr(15)-O(97)#1	2.441(8)
Pr(1)-O(65)	2.566(8)	Pr(15)-O(90)	2.477(9)
Pr(1)-O(9)	2.593(8)	Pr(15)-O(19)#1	2.534(8)
Pr(2)-O(7)	2.435(8)	Pr(15)-O(16)	2.592(8)
Pr(2)-O(5)	2.473(7)	Pr(15)-O(10)	2.598(8)
Pr(2)-O(77)	2.477(8)	Pr(15)-O(85)	2.633(8)
Pr(2)-O(45)	2.494(8)	Pr(15)-O(51)	2.755(8)
Pr(2)-O(57)	2.498(9)	Pr(16)-O(90)	2.423(8)
Pr(2)-O(6)	2.517(8)	Pr(16)-O(54)	2.460(8)
Pr(2)-O(67)	2.539(8)	Pr(16)-O(115)	2.468(9)
Pr(2)-O(65)	2.586(8)	Pr(16)-O(31)	2.487(8)
Pr(2)-O(26)	2.648(8)	Pr(16)-O(110)	2.499(8)
Pr(3)-O(7)	2.416(7)	Pr(16)-O(92)	2.522(9)
Pr(3)-O(82)	2.455(8)	Pr(16)-O(16)	2.577(8)
Pr(3)-O(18)	2.464(8)	Pr(16)-O(116)	2.591(8)
Pr(3)-O(27)	2.478(8)	Pr(16)-O(13)	2.659(7)
Pr(3)-O(5)	2.512(8)	Pr(17)-O(61)	2.402(9)
Pr(3)-O(43)#1	2.514(8)	Pr(17)-O(89)#1	2.458(8)
Pr(3)-O(42)	2.522(8)	Pr(17)-O(103)	2.487(9)
Pr(3)-O(17)	2.543(8)	Pr(17)-O(110)	2.494(8)
Pr(3)-O(60)	2.556(8)	Pr(17)-O(16)	2.536(7)
Pr(4)-O(59)	2.377(9)	Pr(17)-O(97)#1	2.542(9)
Pr(4)-O(5)	2.419(8)	Pr(17)-O(74)	2.544(9)
Pr(4)-O(24)	2.429(8)	Pr(17)-O(88)	2.563(8)
Pr(4)-O(29)	2.462(8)	Pr(17)-O(71)	2.593(9)
Pr(4)-O(10)	2.499(8)	Pr(18)-O(135)	2.413(10)
Pr(4)-O(34)	2.505(8)	Pr(18)-O(136)	2.442(9)
Pr(4)-O(45)	2.883(7)	Pr(18)-O(111)	2.472(9)
Pr(4)-O(128)	2.901(10)	Pr(18)-O(2)	2.49(2)
Pr(5)-O(94)	2.364(9)	Pr(18)-O(23W)	2.535(14)
Pr(5)-O(8)#1	2.468(8)	Pr(18)-O(139)	2.538(10)

Pr(5)-O(76)#1	2.503(9)	Pr(18)-O(47)	2.556(8)
Pr(5)-O(66)	2.503(8)	Pr(18)-O(140)	2.597(11)
Pr(5)-O(22)	2.517(8)	Pr(18)-O(1H)	2.655(11)
Pr(5)-O(27)#1	2.524(8)	Pr(19)-O(25)	2.405(8)
Pr(5)-O(59)#1	2.553(9)	Pr(19)-O(12)	2.411(8)
Pr(5)-O(42)#1	2.564(8)	Pr(19)-O(36)	2.464(8)
Pr(5)-O(83)#1	2.637(9)	Pr(19)-O(118)	2.478(8)
Pr(6)-O(122)	2.448(8)	Pr(19)-O(19)	2.485(8)
Pr(6)-O(32)	2.454(8)	Pr(19)-O(34)#1	2.558(8)
Pr(6)-O(28)	2.480(7)	Pr(19)-O(4)#1	2.605(8)
Pr(6)-O(77)#1	2.513(8)	Pr(19)-O(85)#1	2.675(8)
Pr(6)-O(20)#1	2.522(7)	Pr(19)-O(56)#1	2.738(7)
Pr(6)-O(78)	2.537(9)	Pr(20)-O(122)	2.453(8)
Pr(6)-O(26)#1	2.625(8)	Pr(20)-O(2)	2.47(2)
Pr(6)-O(33)#1	2.640(8)	Pr(20)-O(1H)	2.483(12)
Pr(6)-O(70)	2.653(8)	Pr(20)-O(3)#1	2.495(10)
Pr(7)-O(14)	2.431(8)	Pr(20)-O(135)	2.512(11)
Pr(7)-O(31)	2.451(8)	Pr(20)-O(127)	2.515(9)
Pr(7)-O(24)	2.484(8)	Pr(20)-O(137)	2.535(14)
Pr(7)-O(87)	2.489(8)	Pr(20)-O(32)	2.557(7)
Pr(7)-O(101)	2.492(9)	Pr(20)-O(104)	2.604(11)
Pr(7)-O(13)	2.534(8)	Pr(21)-O(19)	2.411(8)
Pr(7)-O(37)	2.537(8)	Pr(21)-O(74)#1	2.447(9)
Pr(7)-O(21)	2.555(8)	Pr(21)-O(118)	2.489(8)
Pr(7)-O(73)	2.576(8)	Pr(21)-O(100)	2.518(10)
Pr(8)-O(47)	2.458(8)	Pr(21)-O(97)	2.582(9)
Pr(8)-O(136)	2.474(9)	Pr(21)-O(105)#1	2.610(9)
Pr(8)-O(28)#1	2.485(7)	Pr(21)-O(85)#1	2.841(8)
Pr(8)-O(20)	2.492(7)	Pr(21)-Cl(5)	2.976(7)
Pr(8)-O(123)	2.516(10)	Ni(1)-N(12)	2.104(11)
Pr(8)-O(11)	2.518(8)	Ni(2)-N(10)	2.082(9)
Pr(8)-O(113)	2.638(8)	Ni(3)-N(5)	2.076(11)
Pr(8)-O(52)#1	2.654(8)	Ni(4)-N(16)	2.076(9)
Pr(8)-O(9)	2.659(7)	Ni(5)-N(6)	2.117(10)
Pr(9)-O(61)	2.401(9)	Ni(6)-N(4)	2.025(12)
Pr(9)-O(87)	2.482(8)	Ni(7)-N(17)	2.079(10)
Pr(9)-O(8)	2.488(8)	Ni(8)-N(11)	2.080(10)
Pr(9)-O(49)#1	2.495(8)	Ni(9)-N(14)	2.072(11)
Pr(9)-O(93)	2.505(9)	Ni(10)-N(9)	2.112(12)
Pr(9)-O(88)	2.521(8)	Ni(11)-N(18)	2.105(11)
Pr(9)-O(59)	2.538(9)	Ni(12)-N(3)#1	2.092(11)
Pr(9)-O(37)	2.557(7)	Ni(13)-N(15)	2.070(11)
Pr(9)-O(58)	2.579(9)	Ni(14)-N(8)#1	2.134(11)
Pr(10)-O(36)	2.418(8)	Ni(15)-N(1)#1	2.060(10)

Pr(10)-O(63)	2.460(8)	Ni(16)-N(2)	2.078(10)
Pr(10)-O(18)#1	2.464(8)	Ni(17)-N(19)	2.109(12)
Pr(10)-O(39)	2.473(7)	Ni(18)-N(7)	2.104(11)
Pr(10)-O(109)	2.479(8)	Ni(19)-N(20)	2.084(18)
Pr(10)-O(40)	2.515(8)	Ni(19)-Cl(5)	2.326(7)
Pr(10)-O(4)#1	2.537(7)	O(3)-Pr(20)#1	2.495(10)
Pr(10)-O(114)	2.604(9)	O(4)-Pr(10)#1	2.537(7)
Pr(10)-O(17)#1	2.645(8)	O(4)-Pr(14)#1	2.559(7)
Pr(11)-O(47)	2.470(8)	O(4)-Pr(19)#1	2.605(8)
Pr(11)-O(51)	2.487(9)	O(8)-Pr(5)#1	2.468(8)
Pr(11)-O(54)	2.510(8)	O(12)-Pr(15)#1	2.400(7)
Pr(11)-O(90)	2.510(8)	O(12)-Pr(13)#1	2.461(8)
Pr(11)-O(135)	2.531(11)	O(17)-Pr(10)#1	2.645(8)
Pr(11)-O(50)	2.545(8)	O(18)-Pr(10)#1	2.463(8)
Pr(11)-O(123)	2.556(10)	O(19)-Pr(15)#1	2.534(8)
Pr(11)-O(104)	2.558(11)	O(20)-Pr(6)#1	2.522(7)
Pr(11)-O(121)	2.677(9)	O(25)-Pr(13)#1	2.424(8)
Pr(12)-O(39)	2.480(8)	O(26)-Pr(6)#1	2.625(8)
Pr(12)-O(32)	2.485(7)	O(27)-Pr(5)#1	2.524(8)
Pr(12)-O(56)#1	2.516(8)	O(28)-Pr(8)#1	2.485(7)
Pr(12)-O(36)	2.547(7)	O(33)-Pr(6)#1	2.640(8)
Pr(12)-O(78)	2.554(10)	O(34)-Pr(19)#1	2.558(8)
Pr(12)-O(25)	2.573(8)	O(35)-Pr(13)#1	2.592(8)
Pr(12)-O(1H)	2.630(11)	O(42)-Pr(5)#1	2.564(8)
Pr(12)-O(140)	2.629(12)	O(43)-Pr(3)#1	2.514(8)
Pr(12)-O(2)	2.69(2)	O(49)-Pr(9)#1	2.495(8)
Pr(12)-O(98)	2.717(9)	O(52)-Pr(8)#1	2.654(8)
Pr(13)-O(50)	2.394(8)	O(56)-Pr(12)#1	2.515(8)
Pr(13)-O(25)#1	2.424(8)	O(56)-Pr(19)#1	2.738(7)
Pr(13)-O(12)#1	2.461(8)	O(59)-Pr(5)#1	2.553(9)
Pr(13)-O(78)#1	2.559(9)	O(74)-Pr(21)#1	2.447(9)
Pr(13)-O(53)	2.577(8)	O(76)-Pr(5)#1	2.503(9)
Pr(13)-O(35)#1	2.593(8)	O(77)-Pr(6)#1	2.513(8)
Pr(13)-O(123)	2.603(10)	O(78)-Pr(13)#1	2.559(9)
Pr(13)-O(117)	2.765(8)	O(83)-Pr(5)#1	2.637(9)
Pr(13)-Cl(2)	3.1270(7)	O(85)-Pr(19)#1	2.675(8)
Pr(14)-O(94)	2.408(9)	O(85)-Pr(21)#1	2.841(8)
Pr(14)-O(100)	2.473(9)	O(89)-Pr(17)#1	2.458(8)
Pr(14)-O(133)	2.484(9)	O(97)-Pr(15)#1	2.441(8)
Pr(14)-O(40)	2.507(8)	O(97)-Pr(17)#1	2.542(9)
Pr(14)-O(48)	2.538(9)	O(105)-Pr(21)#1	2.610(9)

Table S7 Selected bond angles (°) for compound **2**

O(5)-Pr(4)-O(10)	157.6(3)	O(4)#1-Pr(19)-O(56)#1	76.4(2)
O(24)-Pr(4)-O(10)	91.8(3)	O(85)#1-Pr(19)-O(56)#1	142.12(17)
O(29)-Pr(4)-O(10)	63.4(2)	O(122)-Pr(20)-O(2)	73.7(5)
O(59)-Pr(4)-O(34)	93.9(3)	O(122)-Pr(20)-O(1H)	121.9(3)
O(5)-Pr(4)-O(34)	94.2(3)	O(2)-Pr(20)-O(1H)	55.5(5)
O(24)-Pr(4)-O(34)	155.2(3)	O(122)-Pr(20)-O(3)#1	82.1(2)
O(29)-Pr(4)-O(34)	64.0(3)	O(2)-Pr(20)-O(3)#1	144.7(6)
O(10)-Pr(4)-O(34)	67.4(3)	O(1H)-Pr(20)-O(3)#1	123.9(3)
O(59)-Pr(4)-O(45)	161.5(3)	O(122)-Pr(20)-O(135)	116.8(3)
O(5)-Pr(4)-O(45)	68.8(2)	O(2)-Pr(20)-O(135)	70.9(5)
O(24)-Pr(4)-O(45)	68.0(2)	O(1H)-Pr(20)-O(135)	73.7(4)
O(29)-Pr(4)-O(45)	46.4(2)	O(3)#1-Pr(20)-O(135)	144.3(2)
O(10)-Pr(4)-O(45)	101.6(2)	O(122)-Pr(20)-O(127)	110.7(3)
O(34)-Pr(4)-O(45)	102.0(2)	O(2)-Pr(20)-O(127)	142.8(5)
O(59)-Pr(4)-O(128)	59.9(2)	O(1H)-Pr(20)-O(127)	126.4(3)
O(5)-Pr(4)-O(128)	70.85(19)	O(3)#1-Pr(20)-O(127)	70.0(2)
O(24)-Pr(4)-O(128)	59.5(2)	O(135)-Pr(20)-O(127)	74.8(3)
O(29)-Pr(4)-O(128)	147.2(2)	O(122)-Pr(20)-O(137)	156.2(4)
O(10)-Pr(4)-O(128)	131.56(19)	O(2)-Pr(20)-O(137)	112.5(5)
O(34)-Pr(4)-O(128)	144.8(2)	O(1H)-Pr(20)-O(137)	57.2(3)
O(45)-Pr(4)-O(128)	101.7(2)	O(3)#1-Pr(20)-O(137)	81.0(3)
O(94)-Pr(5)-O(8)#1	76.0(2)	O(135)-Pr(20)-O(137)	86.5(4)
O(94)-Pr(5)-O(76)#1	144.0(3)	O(127)-Pr(20)-O(137)	78.7(4)
O(8)#1-Pr(5)-O(76)#1	68.2(2)	O(122)-Pr(20)-O(32)	68.69(19)
O(94)-Pr(5)-O(66)	88.1(2)	O(2)-Pr(20)-O(32)	70.6(6)
O(8)#1-Pr(5)-O(66)	68.6(3)	O(1H)-Pr(20)-O(32)	69.3(3)
O(76)#1-Pr(5)-O(66)	76.0(2)	O(3)#1-Pr(20)-O(32)	76.8(3)
O(94)-Pr(5)-O(22)	69.1(2)	O(135)-Pr(20)-O(32)	137.1(2)
O(8)#1-Pr(5)-O(22)	124.6(3)	O(127)-Pr(20)-O(32)	146.4(2)
O(76)#1-Pr(5)-O(22)	130.3(2)	O(137)-Pr(20)-O(32)	91.2(3)
O(66)-Pr(5)-O(22)	68.6(3)	O(122)-Pr(20)-O(104)	50.7(3)
O(94)-Pr(5)-O(27)#1	72.3(2)	O(2)-Pr(20)-O(104)	81.5(5)
O(8)#1-Pr(5)-O(27)#1	131.0(3)	O(1H)-Pr(20)-O(104)	132.3(4)
O(76)#1-Pr(5)-O(27)#1	136.01(19)	O(3)#1-Pr(20)-O(104)	102.8(2)
O(66)-Pr(5)-O(27)#1	144.1(3)	O(135)-Pr(20)-O(104)	73.4(3)
O(22)-Pr(5)-O(27)#1	76.2(3)	O(127)-Pr(20)-O(104)	75.3(3)
O(94)-Pr(5)-O(59)#1	85.4(2)	O(137)-Pr(20)-O(104)	150.5(4)
O(8)#1-Pr(5)-O(59)#1	68.2(3)	O(32)-Pr(20)-O(104)	118.2(2)
O(76)#1-Pr(5)-O(59)#1	84.6(2)	O(19)-Pr(21)-O(74)#1	97.6(2)
O(66)-Pr(5)-O(59)#1	136.6(3)	O(19)-Pr(21)-O(118)	67.5(2)
O(22)-Pr(5)-O(59)#1	144.7(3)	O(74)#1-Pr(21)-O(118)	138.4(3)
O(27)#1-Pr(5)-O(59)#1	72.9(3)	O(19)-Pr(21)-O(100)	97.0(2)
O(77)#1-Pr(6)-O(20)#1	72.60(17)	O(19)-Pr(21)-Cl(5)	144.0(2)
O(122)-Pr(6)-O(78)	82.6(3)	O(74)#1-Pr(21)-Cl(5)	107.5(2)

O(32)-Pr(6)-O(78)	70.5(2)	O(118)-Pr(21)-Cl(5)	76.59(19)
O(28)-Pr(6)-O(78)	74.0(2)	O(100)-Pr(21)-Cl(5)	66.5(2)
O(77)#1-Pr(6)-O(78)	151.3(3)	O(97)-Pr(21)-Cl(5)	146.4(2)
O(20)#1-Pr(6)-O(78)	81.2(2)	O(105)#1-Pr(21)-Cl(5)	76.2(2)
O(122)-Pr(6)-O(26)#1	146.76(19)	N(13)#1-Pr(21)-Cl(5)	67.3(2)
O(32)-Pr(6)-O(26)#1	76.8(2)	O(85)#1-Pr(21)-Cl(5)	113.19(17)
O(28)-Pr(6)-O(26)#1	133.6(2)	O(37)-Ni(1)-O(72)	98.5(2)
O(77)#1-Pr(6)-O(26)#1	69.05(17)	O(37)-Ni(1)-O(58)	85.7(3)
O(20)#1-Pr(6)-O(26)#1	71.5(2)	O(72)-Ni(1)-O(58)	89.7(3)
O(78)-Pr(6)-O(26)#1	91.8(2)	O(37)-Ni(1)-O(73)	84.9(2)
O(122)-Pr(6)-O(33)#1	76.18(19)	O(72)-Ni(1)-O(73)	173.9(3)
O(32)-Pr(6)-O(33)#1	71.4(2)	O(58)-Ni(1)-O(73)	85.4(3)
O(28)-Pr(6)-O(33)#1	130.2(2)	O(37)-Ni(1)-O(41)	97.2(3)
O(77)#1-Pr(6)-O(33)#1	62.67(17)	O(72)-Ni(1)-O(41)	95.4(2)
O(20)#1-Pr(6)-O(33)#1	135.1(2)	O(58)-Ni(1)-O(41)	173.7(3)
O(78)-Pr(6)-O(33)#1	140.7(2)	O(73)-Ni(1)-O(41)	89.3(2)
O(26)#1-Pr(6)-O(33)#1	88.4(2)	O(37)-Ni(1)-N(12)	160.9(3)
O(122)-Pr(6)-O(70)	64.62(19)	O(72)-Ni(1)-N(12)	95.3(4)
O(32)-Pr(6)-O(70)	124.4(2)	O(58)-Ni(1)-N(12)	81.2(3)
O(28)-Pr(6)-O(70)	63.3(2)	O(73)-Ni(1)-N(12)	80.3(4)
O(77)#1-Pr(6)-O(70)	66.87(18)	O(41)-Ni(1)-N(12)	94.6(3)
O(20)#1-Pr(6)-O(70)	99.3(2)	O(28)-Ni(2)-O(70)	84.1(3)
O(78)-Pr(6)-O(70)	130.5(2)	O(28)-Ni(2)-O(35)#1	98.0(3)
O(26)#1-Pr(6)-O(70)	135.7(2)	O(70)-Ni(2)-O(35)#1	177.9(3)
O(33)#1-Pr(6)-O(70)	67.6(2)	O(28)-Ni(2)-O(52)	83.9(3)
O(14)-Pr(7)-O(31)	119.9(3)	O(70)-Ni(2)-O(52)	83.6(3)
O(14)-Pr(7)-O(24)	69.5(3)	O(35)#1-Ni(2)-O(52)	96.9(3)
O(31)-Pr(7)-O(24)	143.6(3)	O(28)-Ni(2)-N(10)	161.3(3)
O(14)-Pr(7)-O(87)	132.08(19)	O(70)-Ni(2)-N(10)	82.6(3)
O(31)-Pr(7)-O(87)	75.78(19)	O(35)#1-Ni(2)-N(10)	95.4(3)
O(24)-Pr(7)-O(87)	74.11(19)	O(52)-Ni(2)-N(10)	81.6(3)
O(14)-Pr(7)-O(101)	68.85(19)	O(28)-Ni(2)-O(53)	97.8(3)
O(31)-Pr(7)-O(101)	132.3(2)	O(70)-Ni(2)-O(53)	96.8(3)
O(24)-Pr(7)-O(101)	84.10(19)	O(35)#1-Ni(2)-O(53)	82.7(3)
O(87)-Pr(7)-O(101)	136.7(3)	O(52)-Ni(2)-O(53)	178.3(3)
O(14)-Pr(7)-O(13)	72.8(3)	N(10)-Ni(2)-O(53)	96.8(3)
O(31)-Pr(7)-O(13)	70.3(3)	O(14)-Ni(3)-O(15)	83.8(3)
O(24)-Pr(7)-O(13)	81.1(3)	O(14)-Ni(3)-O(44)	95.9(3)
O(87)-Pr(7)-O(13)	71.68(19)	O(15)-Ni(3)-O(44)	91.8(3)
O(101)-Pr(7)-O(13)	141.60(19)	O(14)-Ni(3)-O(101)	86.0(2)
O(14)-Pr(7)-O(37)	131.9(3)	O(15)-Ni(3)-O(101)	87.6(2)
O(31)-Pr(7)-O(37)	107.8(3)	O(44)-Ni(3)-O(101)	177.9(3)
O(24)-Pr(7)-O(37)	75.9(3)	O(14)-Ni(3)-N(5)	161.3(3)
O(87)-Pr(7)-O(37)	63.24(19)	O(15)-Ni(3)-N(5)	82.1(3)

O(101)-Pr(7)-O(37)	75.4(2)	O(44)-Ni(3)-N(5)	96.8(3)
O(13)-Pr(7)-O(37)	133.3(3)	O(101)-Ni(3)-N(5)	81.1(4)
O(14)-Pr(7)-O(21)	68.3(3)	O(14)-Ni(3)-O(131)	96.4(2)
O(31)-Pr(7)-O(21)	66.2(3)	O(15)-Ni(3)-O(131)	179.0(2)
O(24)-Pr(7)-O(21)	137.6(3)	O(44)-Ni(3)-O(131)	87.2(2)
O(87)-Pr(7)-O(21)	141.65(19)	O(101)-Ni(3)-O(131)	93.4(3)
O(101)-Pr(7)-O(21)	77.4(2)	N(5)-Ni(3)-O(131)	97.9(4)
O(13)-Pr(7)-O(21)	90.3(3)	O(65)-Ni(4)-O(64)	99.2(3)
O(37)-Pr(7)-O(21)	133.1(3)	O(65)-Ni(4)-O(95)	84.5(2)
O(14)-Pr(7)-O(73)	125.31(19)	O(64)-Ni(4)-O(95)	88.5(2)
O(31)-Pr(7)-O(73)	70.72(19)	O(65)-Ni(4)-O(67)	85.2(3)
O(24)-Pr(7)-O(73)	135.97(19)	O(64)-Ni(4)-O(67)	170.2(3)
O(87)-Pr(7)-O(73)	102.5(3)	O(95)-Ni(4)-O(67)	83.3(2)
O(101)-Pr(7)-O(73)	68.5(3)	O(65)-Ni(4)-O(68)	97.0(3)
O(13)-Pr(7)-O(73)	140.81(19)	O(64)-Ni(4)-O(68)	97.9(3)

Table S8 Hydrogen bond interactions in compound **2**

D-H···A	d(D···H) /Å	d(H···A)/ Å	d(D···A)/Å	D-H···A (°)
N1-H1A··O41	0.91	2.29	3.184(13)	168
N4-H4A··O125	0.91	2.23	2.936(15)	134
N10-H10A··O117	0.91	2.13	2.952(12)	150
N15-H15C··O68	0.91	2.12	2.916(14)	145
N18-H18A··O84	0.91	2.16	2.994(14)	152
C3-H3B··O72	0.97	2.22	3.181(17)	169
C15-H15A··O6W	0.97	2.48	3.26(3)	138
C20-H20B··O75	0.97	2.54	3.471(16)	161
C39-H39A··O108	0.97	2.44	3.250(14)	141
C57-H57B··O64	0.97	2.4	3.158(17)	135
C60-H60A··O64	0.97	2.24	3.096(16)	147
C71-H71B··O81	0.97	2.33	3.148(16)	141
C77-H77A··O20W	0.97	2.44	3.00(4)	116