Supporting Information

"Three function in one": multifunctional rare-earth cyamelurates with magnetism, luminescence, and giant optical nonlinearity

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Experimental Procedures

1. Synthesis

All reagents were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd., and used directly, including melamine ($C_3H_6N_6$, Aladdin, 99%), $YCl_3·6H_2O$ (Aladdin, 99.99%)/$GdCl_3·6H_2O$ (Aladdin, 99.99%)/$LuCl_3·6H_2O$ (Aladdin, 99.99%), and LiOH (Aladdin, 99%). Potassium cyamelurate was prepared before.[1] The potassium cyamelurate (1 mmol, 0.275 g), LiOH (0.5 mmol, 0.021g), and $YCl_3·6H_2O$ (1 mmol, 0.303 g)/$GdCl_3·6H_2O$ (1 mmol, 0.372 g)/$LuCl_3·6H_2O$ (1 mmol, 0.389 g) were solved in 40 mL deionized water, and the solution was then heated to boiling. Colourless transparent crystals appeared at the bottom of the beaker when cooled to room temperature.

2. Characterization

Single crystal X-ray determination

The single-crystal X-ray diffraction data for $RE(H_{1.5}C_6N_7O_3)_2·10H_2O$ (RE= Y, Gd, Lu) was collected on Bruker SMART APEX II 4K CCD single crystal diffractometer at 298 K with Mo Kα radiation (λ = 0.71073 Å). APEX3 software was applied to perform data collection, reduction, and cell refinement. The crystal structures were determined with the ShelXT by intrinsic phasing method and refined with the ShelXTL package using Olex2.[2-4] No higher symmetry was found by the adoption of PLATON30.[5] Table S1-S12 lists the detailed crystallographic data for $RE(H_{1.5}C_6N_7O_3)_2·10H_2O$ (RE= Y, Gd, Lu).

Powder X-ray diffraction

Powder X-ray diffraction patterns were collected by a Smart Lab 9 kW X-ray diffractometer under Cu Kα radiation (λ = 1.5418 Å) with the 2θ scan range from 5° to 80°.

Infrared spectroscopy

A Nicolet iS50 FT-IR spectrometer with attenuated total reflection (ATR) covering the spectral range from 500 cm^{-1} to 4000 cm^{-1} was used to record the infrared spectra of crystals.

Thermal analysis

The thermal analysis was carried out on a EVO2 G-TG thermal analyzer instrument and NETZSCH 209 F3 under N_2 atmosphere. The temperature varied from 40 °C to 900 °C with the heating/cooling rate of 10 °C min^{-1}.

UV-vis-NIR diffuse reflectance spectrum

A UH4150 UV–vis–NIR spectrophotometer with $BaSO_4$ as the standard of 100 % was used to collect the diffuse reflectance spectra. The reflection spectrum was converted by the Kubelka–Munk function, $F(R) = (1-R)^2/2R$, where R is the reflectance coefficient.[6,7] The corresponding band gaps were deduced by straightforward extrapolation method.[8] The transmittance spectrum was also recorded on a UH4150 UV−vis-NIR spectrophotometer.

Power SHG measurement

SHG responses of $RE(H_{1.5}C_6N_7O_3)_2·10H_2O$ (RE= Y, Gd, Lu) were measured on a Q-switched Nd:YAG laser under 1064 nm incident light. The crystalline samples were ground and sieved into different sizes: 50 - 74 μm, 74 - 100 μm, 100 - 154 μm, 154 - 200 μm, and 200 - 250 μm. KH_2PO_4 (KDP) was used as the reference.

Fluorescence measurement

An Edinburgh fluorescence spectrometer was used to collect fluorescence spectra. The incident source was Xenon lamp light (280−310 nm). The wavelength step (0.1 nm) and dwell time (0.02 s) were set in the experiment.

Magnetic susceptibility

The magnetic susceptibilities of the as-prepared crystal samples were measured using a Quantum Design Physical Property Measurement System (PPMS). The crystal samples were secured to a quartz rod using GE varnish. The temperature dependence of the magnetic susceptibility (χ) was measured at B = 0.5 T across a broader range of 2–300 K. Magnetization (M) versus magnetic field (B) curves were obtained at 2 K over a field range of 0–14 T.

In-plane birefringence measurement

The in-plane birefringence was estimated by A Nikon Eclipse polarizing microscope E200MV POL with a halogen lamp 6 V–30 W (PHILIPS 5761), and the value was calculated as follows: $\Delta R = \Delta n \times T$, where ΔR, Δn, and T respectively denote the optical path difference, the in-plane birefringence, and the crystal thickness.[9] The value of the optical range difference was determined from the interferometric chromatogram. The crystal thickness was measured on a Bruker SMART APEX II single crystal diffractometer.

3. Calculation Method

The first principles calculations for $RE(H_{1.5}C_6N_7O_3)_2·10H_2O$ (RE= Y, Gd, Lu) carried out by CASTEP package based on density functional theory are similar to metal cyanurates previously reported.[10-12] To ensure the accuracy of the calculated results, the energy cutoff (850 eV) and a Monkhorst-Pack *k*-point meshes (3×1×4) in the first Brillouin zone were adopted.[13] Generalized gradient

approximation (GGA) Perdew-Burke-Ernzerhof (PBEsol) functional was used to describe the exchange–correlation functionals and the ion-electron interactions for all constituent atoms were modeled by the norm-conserving pseudopotentials.[14-15] Based on the electronic structures including spin-orbital coupling effect, the refractive indices and corresponding birefringence values were derived. Besides, phonon dispersion, infrared (IR), and Raman spectra were obtained using the linear response method.[16]

Results and Discussion

Figure S1. Powder X-ray diffraction patterns and crystal pictures of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, (b) $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, and (c) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

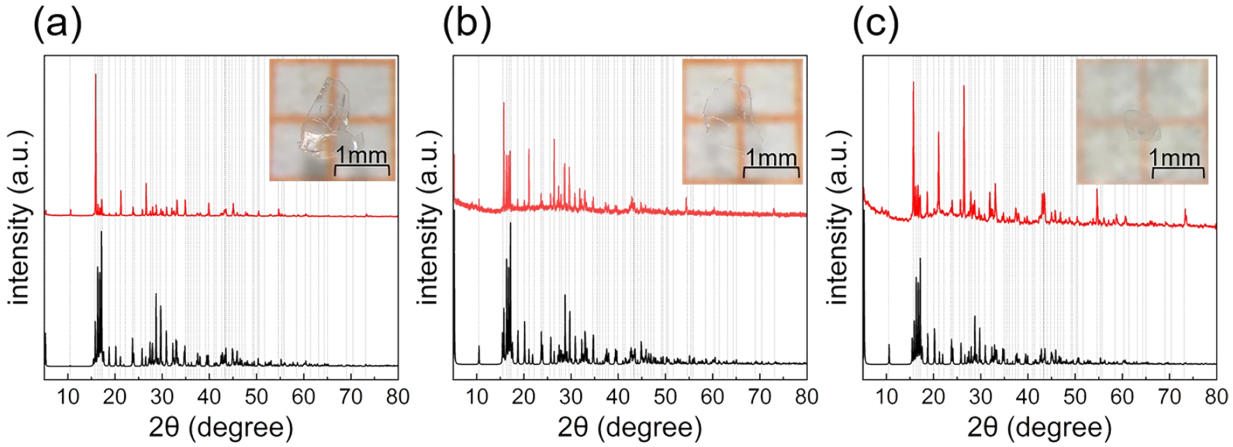

Figure S2. Thermal analysis of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, (b) $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, and (c) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

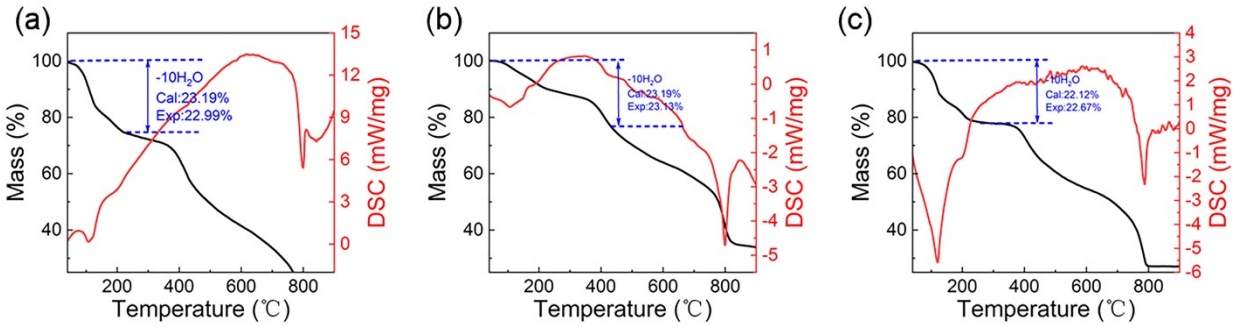

Figure S3. XRD patterns of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, (b) $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, and (c) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$ after six months.

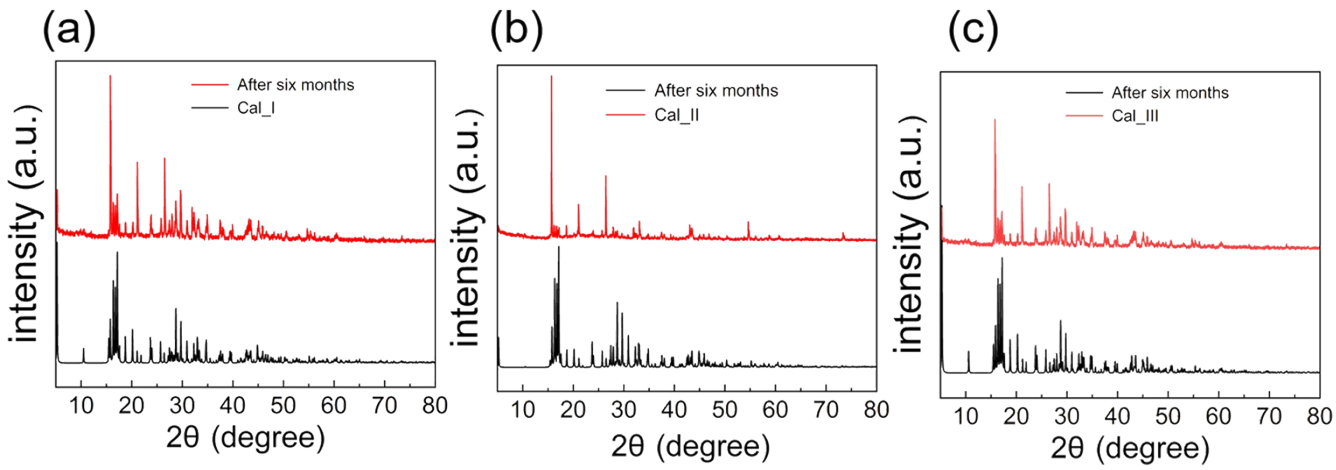

Figure S4. IR spectra of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, (b) $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, and (c) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

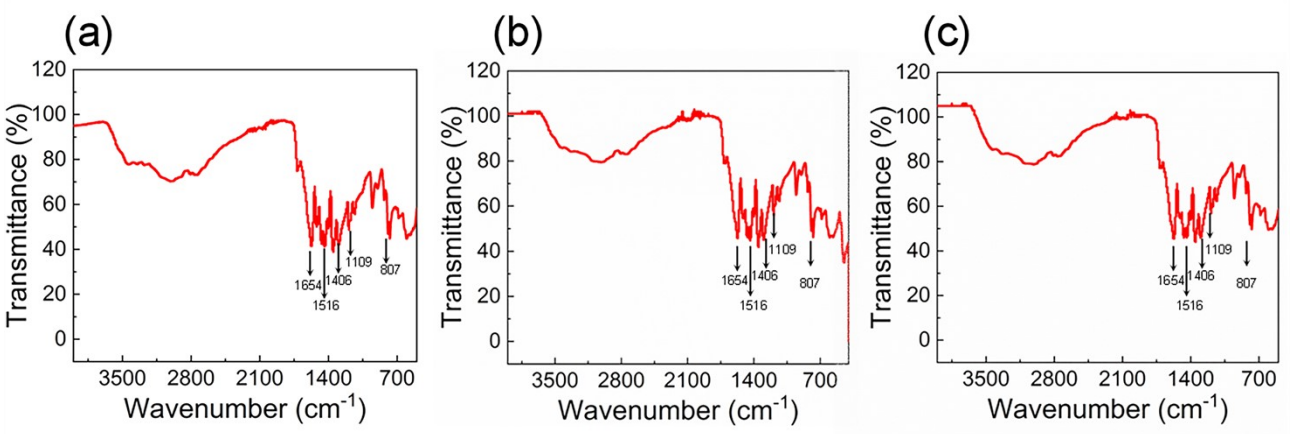

Figure S5. UV/Visible-near infrared diffuse reflectance spectra of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, (b) $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, and (c) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

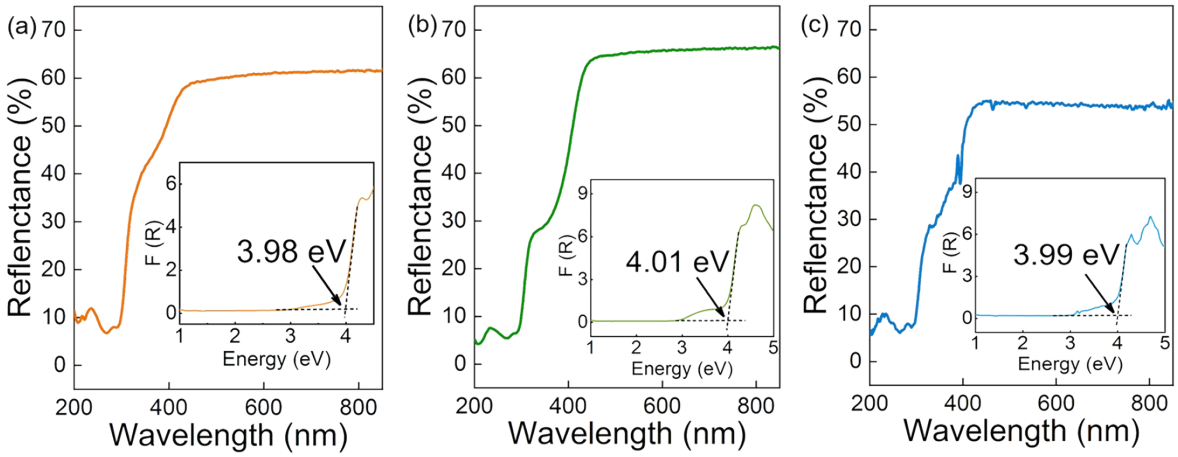

Figure S6. Photoluminescent measurement of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$ and (b) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

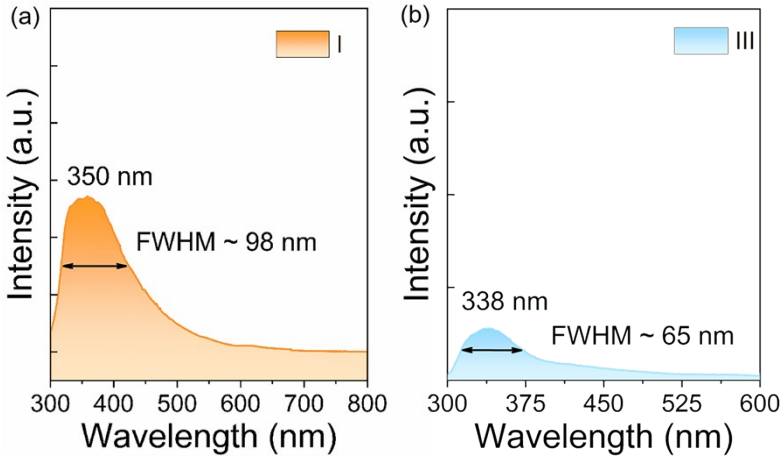

Figure S7. Calculated band structures of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$ and (b) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

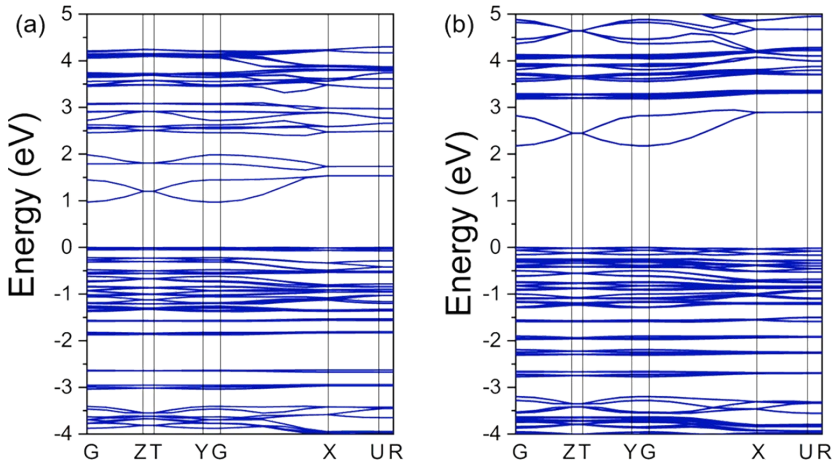

Figure S8. DOS and partial DOS of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$ and (b) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

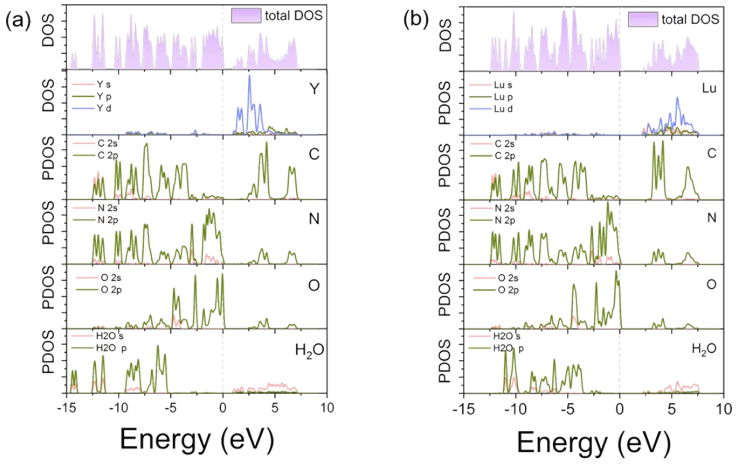

Figure S9. The calculated birefringence of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$ and (b) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

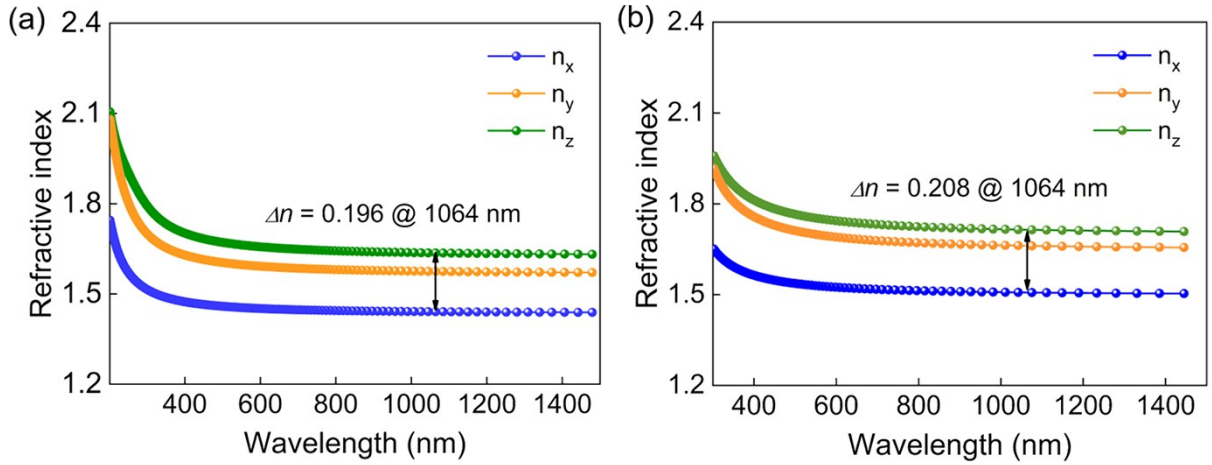

Figure S10. Birefringence measurement of (a) $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, (b) $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$, and (c) $Lu(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

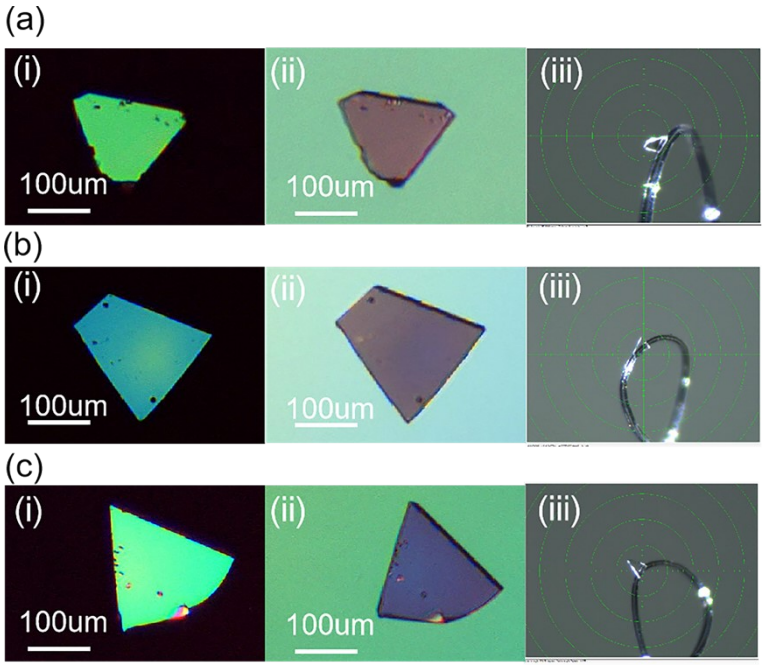

Table S1. Fractional atomic coordinates (x10^4) and equivalent isotropic displacement parameters(Å^{2}x10^3) for $Y(H_{1.5}C_6N_7O_3)_2 \cdot 10H_2O$.

Atom	x	y	z	U (eq)
Y1	7500	2500	6438.4(15)	23.8(5)
O7	6515.2(10)	11596(11)	403(6)	10.5(13)
O1	6738.3(10)	9142(11)	2042(6)	13.2(13)
O2	6248.0(9)	-40(11)	3746(6)	8.0(14)
O3	7184.4(12)	1929(15)	5728(8)	22.2(16)
N7	6880.7(12)	1126(14)	5057(8)	10.3(15)
N4	6730.0(11)	3662(12)	3799(7)	6.4(14)
N6	6559.6(11)	581(13)	4416(7)	6.2(14)
O6	7625.1(13)	5783(14)	7292(8)	25.4(18)
N3	6399.5(11)	3093(13)	3146(7)	6.9(14)
O8	7992.7(14)	7228(14)	6753(7)	25.6(19)
N2	6903.2(12)	6874(14)	3251(8)	11.9(15)
N1	6574.8(11)	6114(12)	2582(7)	7.3(14)
N5	7052.6(12)	4402(15)	4486(8)	12.6(16)
O5	7719.7(12)	1141(14)	7960(10)	30(2)
C5	6729.7(13)	1755(14)	4452(8)	6.1(15)
C1	6744.8(13)	7484(14)	2589(8)	7.5(16)
O4	7539.9(16)	-184(17)	4943(9)	34(2)
C3	6899.6(12)	5028(14)	3850(10)	6.6(16)
C4	6394.6(13)	1149(14)	3765(7)	6.7(16)
C2	6560.6(13)	4243(15)	3186(8)	6.7(16)
C6	7042.6(14)	2502(15)	5086(8)	10.9(18)

Table S2. Anisotropic displacement parameters ($Å^2×10^3$) for $Y(H_{1.5}C_6N_7O_3)_2·10H_2O$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y1	18.6(7)	28.2(8)	24.6(7)	0	0	-1.2(6)
O7	11(3)	8(3)	13(3)	-1(2)	2 (3)	-2(2)
O1	16(3)	8 (3)	16 (3)	1(3)	3 (3)	-4(3)
O2	6 (3)	9 (3)	9 (4)	0(2)	-2(2)	-2(2)
O3	11(3)	31(4)	25(4)	-1(3)	-10(3)	2 (3)
N7	7(3)	13(4)	10(3)	-5(3)	-5 (3)	2(3)
N4	2(3)	8(3)	9 (3)	-2(3)	-1(3)	-2(2)
N6	4(3)	7(3)	8(3)	2 (3)	0(3)	-1(3)
O6	19(4)	22(4)	35 (5)	0 (3)	9(4)	-6(3)
N3	7(2)	7(2)	7(2)	1 (2)	-1(2)	1 (2)
O8	32(5)	22 (4)	23 (5)	7 (3)	-6(3)	-10(3)
N2	10(2)	10(2)	16(3)	-3(2)	1(2)	-1(2)
N1	5 (3)	10(3)	8 (3)	1(3)	0(3)	-3(3)
N5	3 (3)	16(4)	19(4)	-6(3)	-4(3)	-1(3)
O5	12(4)	19(4)	59(6)	8(4)	-3 (4)	-8(3)
C5	5(3)	7(2)	6 (2)	-1(2)	1 (2)	0 (2)
C1	5(3)	8(3)	9 (3)	-3(2)	2(2)	-2(2)
O4	34(5)	38(5)	28(5)	3 (4)	7 (4)	-3(4)
C3	5 (2)	6(2)	8(3)	-3(2)	-2(2)	-1(2)
C4	6(4)	10(4)	4 (4)	0 (3)	4 (3)	-2(3)
C2	5 (3)	7 (3)	7(2)	0(2)	0(2)	0(2)
C6	9 (3)	14(3)	10 (3)	0(2)	-1(2)	2 (2)

Table S3. Selected bond lengths for $Y(H_{1.5}C_6N_7O_3)_2 \cdot 10H_2O$.

Bond	Length (Å)	Bond	Length (Å)
Y1-O3	2.295(8)	N4-C5	1.349(11)
Y1-O31	2.295(8)	N4-C3	1.380(11)
Y1-O61	2.387(9)	N4-C2	1.386(12)
Y1-O6	2.387(9)	N6-C5	1.290(12)
Y1-O51	2.432(10)	N6-C4	1.358(13)
Y1-O5	2.432 (10)	N3-C4	1.323(13)
Y1-O4	2.391 (10)	N3-C2	1.415(11)
Y1-O41	2.391(10)	N2-C1	1.342(12)
O1-C1	1.194(12)	N2-C3	1.316(13)
O2-C4	1.223(11)	N1-C1	1.353(13)
O3-C6	1.253(13)	N1-C2	1.349(11)
N7-C5	1.287(12)	N5-C3	1.380(11)
N7-C6	1.375 (12)	N5-C6	1.386(12)

[1]3/2-X,1/2-Y,+Z.

Table S4. Selected bond angles for $Y(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

Angle	(°)	Angle	(°)
O3-Y1-O31	138.4(5)	C6-O3-Y1	150.0(8)
O31-Y1-O6[1]	126.7(3)	C5-N7-C6	116.8(9)
O3-Y1-O6[1]	72 .2(3)	C5-N4-C3	118.5 (7)
O31-Y1-O6	72 .2(3)	C2-N4-C5	119.4(7)
O3-Y1-O6	126.7(3)	C2-N4-C3	122.0(8)
O3-Y1-O51	75.4(3)	C5-N6-C4	124.1(8)
O31-Y1-O51	139.6(3)	C2-N3-C4	118.0(8)
O3-Y1-O5	139.6(3)	C3-N2-C1	120.8(8)
O31-Y1-O5	75.4(3)	C2-N1-C1	124.0(7)
O31-Y1-O4[1]	75.1(3)	C3-N5-C6	119.6(8)
O3-Y1-O4	75.1(3)	N7-C5-N4	122.9(8)
O3-Y1-O4[1]	75 .3 (3)	N7-C5-N6	121.5(9)
O31-Y1-O4	75 .3 (3)	N6-C5-N4	115.6(8)
O6-Y1-O6[1]	131.6(4)	O1-C1-N2	123.8(8)
O6-Y1-O5	77.3(3)	O1-C1-N1	118.1(8)
O6[1]-Y1-O51	77.3(3)	N2-C1-N1	118.1(8)
O6-Y1-O51	68 .3(3)	N2-C3-N4	119.9(8)

[1]3/2-X,1/2-Y,+Z

Table S5. Fractional atomic coordinates (x10^4) and equivalent isotropic displacement parameters(Å^{2}x10^3) for $Gd(H_{1.5}C_6N_7O_3)_2 \cdot 10H_2O$.

Atom	x	y	z	U (eq) [a]
Gd1	5000	5000	3584.0(12)	30.7(3)
N4	5770.2(13)	3907(15)	6201(9)	10.9(18)
N3	5596.8(15)	752(18)	6743(10)	18(2)
O2	5764.4(14)	-1605(15)	7935(9)	22.8(19)
O3	6253.6(13)	7538(17)	6180(20)	23(2)
N6	5924.7(14)	1437(16)	7383(9)	14.3(19)
N2	5620.5(15)	6445(18)	4941(10)	18(2)
O1	5317.3(16)	5670(20)	4318(11)	35(2)
N5	5942.5(16)	6931(18)	5569(10)	16(2)
N1	5449.3(16)	3210(19)	5511(10)	20(2)
O6	4873.4(19)	1690(20)	2697(12)	42(3)
O5	4773.3(16)	6368(19)	2068(13)	44(3)
C2	5602.8(16)	2560(20)	6180(20)	12(2)
C1	5461(2)	5090(20)	4919(12)	20(3)
N7	6102.8(15)	4443(18)	6817(9)	16.2(19)
C3	5770.6(16)	5792(18)	5533(10)	11(2)
O4	4952(3)	7780(30)	5046(14)	52(4)
C6	6105.6(16)	6367(18)	6192(11)	14(2)
C4	5754(2)	131(19)	7358(12)	18(2)
C5	5938.9(17)	3320(20)	6782(10)	13(2)
O7	4512(3)	170(20)	3257(13)	48(4)
O8	5981.0(13)	10938(16)	4566(9)	24(2)

[a] U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} ten

Table S6. Anisotropic displacement parameters ($Å^2×10^3$) for $Gd(H_{1.5}C_6N_7O_3)_2·10H_2O$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Gd1	21.0(5)	37.5(5)	33.4(5)	0	0	-1.8(5)
N4	11(4)	8(4)	14(5)	1(4)	-3(4)	-2(3)
N3	16(5)	11(4)	26(5)	3 (4)	-3(4)	-4(4)
O2	27 (5)	9(4)	33(5)	8(4)	-2(4)	-5(4)
O3	13(3)	24(4)	33(7)	3(4)	1(6)	-8(4)
N6	10(4)	15(5)	18(5)	6(4)	-4(4)	-3(4)
N2	13(4)	20(5)	21(5)	3(4)	-4(4)	-1(4)
O1	20(5)	43(6)	42(6)	16(5)	-13 (5)	-6(5)
N5	14(5)	14(5)	21 (5)	3 (4)	-2(4)	-4(4)
N1	10(4)	22(5)	27(5)	5 (5)	-6(4)	-1(4)
O6	35(6)	32(6)	59(8)	-4(6)	10(5)	2(5)
O5	23(5)	29(6)	79(10)	10(6)	-12(6)	-12(4)
C2	8(4)	16(4)	12(7)	-4(4)	1(6)	1(4)
C1	11(6)	26(7)	22(6)	-4(5)	0(5)	2 (4)
N7	13 (5)	17(5)	19(5)	2(4)	-3(4)	-4(4)
C3	13 (5)	10(5)	11(5)	4(5)	2(4)	3(4)
O4	46(8)	59(9)	51(8)	-11(7)	12(7)	-16(7)
C6	12(5)	15(5)	14(5)	1(4)	2(4)	-5(4)
C4	16(6)	17(6)	20(6)	-2(5)	5(5)	-4(4)
C5	9(5)	15(5)	14(5)	-1(5)	0(4)	-1(4)
O7	52(8)	31(7)	60(11)	4(6)	1(6)	-14(5)
O8	18(4)	22(5)	31(5)	8(4)	9(4)	0(4)

Table S7. Selected bond lengths for $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

Bond	Length (Å)	Bond	Length (Å)
Gd1-O1	2.340(11)	O2-C4	1.262(16)
Gd1-O1[1]	2.340(10)	O3-C6	1.230(14)
Gd1-O6[1]	2.434(13)	N6-C4	1.404(15)
Gd1-O6	2.434(13)	N6-C5	1.357(16)
Gd1-O5	2.480(13)	N2-C1	1.362(16)
Gd1-O5[1]	2.480(13)	N2-C3	1.288(15)
Gd1-O4	2.435(15)	O1-C1	1.245(17)
Gd1-O4[1]	2.434(15)	N5-C3	1.354(16)
N4-C2	1.401(14)	N5-C6	1.362(15)
N4-C3	1.395(15)	N1-C2	1.354(19)
N4-C5	1.371(15)	N1-C1	1.347(17)
N3-C2	1.29(2)	N7-C6	1.388(15)
N3-C4	1.334(18)	N7-C5	1.303(16)
Gd1-O1	2.340(11)	O2-C4	1.262(16)

[1]1/2-X,1/2-Y,+Z.

Table S8. Selected bond angles for $Gd(H_{1.5}C_6N_7O_3)_2{\cdot}10H_2O$.

Angle	(°)	Angle	(°)
O1-Gd1-O1[1]	137.2(6)	C3-N4-C2	118.8(11)
O1[1]-Gd1-O6[1]	128.4(4)	C5-N4-C2	121.5(11)
O1[1]-Gd1-O6	71.8(4)	C5-N4-C3	119.4(9)
O1-Gd1-O6[1]	71.8(4)	C2-N3-C4	119.6(11)
O1-Gd1-O6	128.4(4)	C5-N6-C4	122.4(10)
O1-Gd1-O5	139.8(4)	C3-N2-C1	116.2(11)
O1[1]-Gd1-O5[1]	139.8(4)	C1-O1-Gd1	149.9(10)
O1-Gd1-O5[1]	75.8(4)	C3-N5-C6	125.2(11)
O1[1]-Gd1-O5[1]	75.8(4)	C1-N1-C2	120.2(12)
O1[1]-Gd1-O4	75.3(5)	N3-C2-N4	121.6(13)
O1[1]-Gd1-O4[1]	75.2(5)	N3-C2-N1	121.5(11)
O1-Gd1-O4[1]	75.3(5)	N1-C2-N4	116.9(14)
O1-Gd1-O4	75.2(5)	O1-C1-N2	116.8(12)
O6[1]-Gd1-O6	129.9(7)	O1-C1-N1	119.1(12)
O6-Gd1-O5[1]	68.4(4)	N1-C1-N2	124.1(12)
O6-Gd1-O5	76.5(4)	C5-N7-C6	116.5(10)
O6[1]-Gd1-O5	68.4(4)	N2-C3-N4	123.7(10)
O6[1]-Gd1-O5[1]	76.5(4)	N2-C3-N5	121.9(11)
O6[1]-Gd1-O4[1]	75.9(5)	N2-C3-N4	114.4(10)
O6-Gd1-O4[1]	75.9(5)	O3-C6-N5	120.1(12)
O6[1]-Gd1-O4	146.7(5)	O3-C6-N7	121.0(13)
O6-Gd1-O5	146.7(5)	N5-C6-N7	119.0(10)
O5[1]-Gd1-O5	89.4(7)	N3-C4-N6	119.9(11)
O4[1]-Gd1-O5	144.8(4)	O2-C4-N3	124.8(11)
O4[1]-Gd1-O5[1]	100.1(6)	O2-C4-N6	115.3(12)
O4-Gd1-O51	144.8(4)	N6-C5-N4	114.8(10)
O4-Gd1-O5	100.1(6)	N7-C5-N4	125.4(11)
O4[1]-Gd1-O4	91.4(8)	N7-C5-N6	119.7(11)

[1]1-X,1-Y,+Z

Table S9. Fractional atomic coordinates (x10^4) and equivalent isotropic displacement parameters(Å^{2}x10^3) for Lu($H_{1.5}C_6N_7O_3)_2$·$10H_2O$.

Atom	x	y	z	U (eq)
Lu1	5000	5000	3568.5(12)	24.5(3)
N4	5767.5(13)	3877(14)	6177(8)	5.4(16)
O1	5311.5(14)	5625(19)	4277(10)	26(2)
O2	5761.0(13)	-1606(15)	7913(8)	17.1(17)
N1	5615.5(14)	6411(17)	4917(9)	12.9(19)
N6	5593.6(15)	721(17)	6721(10)	14.8(19)
O3	6252.2(13)	7553(16)	6171(19)	19(2)
N3	5444.1(15)	3173(18)	5494(10)	15(2)
N7	5923.0(14)	1429(15)	7363(9)	9.5(18)
C5	5598.9(14)	2530(18)	6151(17)	8(2)
O5	4873.9(18)	1723(19)	2703(11)	31(2)
C1	5454.8(19)	5029(17)	4879(11)	13(2)
O6	4783.7(16)	6303(18)	2099(14)	40(3)
C2	5767.8(16)	5770(18)	5500(9)	7.0(19)
N2	5939.2(15)	6920(18)	5546(9)	11.2(18)
N5	6100.8(14)	4442(17)	6795(9)	10.9(18)
C6	5752.5(19)	102(16)	7347(11)	11(2)
O4	4959(2)	7670(30)	5007(14)	46(4)
C3	6104.6(16)	6362(17)	6175(10)	9.3(19)
C4	5936.7(17)	3320(20)	6745(10)	9(2)
O7	5981.5(13)	10908(15)	4534(8)	18.1(18)
O8	5495(2)	9785(17)	3250(11)	34(3)

Table S10. Anisotropic displacement parameters ($Å^2×10^3$) for $Lu(H_{1.5}C_6N_7O_3)_2·10H_2O$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Lu1	15.8(4)	28.9(4)	28.7(4)	0	0	-0.8(3)
N4	2(4)	4(4)	10(4)	0(3)	-3(3)	0(3)
O1	11(4)	35(5)	34(5)	9(5)	-12(4)	-4(4)
O2	17(2)	16(2)	18(2)	1.4(14)	-0.3(14)	-0.3(14)
N1	6(4)	17(5)	16(5)	4(4)	-5(3)	3(4)
N6	15(5)	5(4)	25(5)	3(4)	-3(4)	-3(4)
O3	9(3)	22(4)	25(7)	5(4)	0(5)	-9(3)
N3	9(4)	13(5)	24(5)	4(4)	-10(4)	-5(4)
N7	8(4)	9(4)	12(4)	7(4)	-1(3)	-3(3)
C5	6(3)	8(3)	9(3)	-2(2)	0(3)	1(2)
O5	29(6)	21(5)	41(6)	0(5)	11(5)	5(5)
C1	7(5)	18(6)	15(6)	-3(4)	-5(4)	-1(4)
O6	17(5)	22(5)	81(10)	6(6)	-6(6)	-9(4)
C2	8(5)	6(4)	7(5)	4(4)	0(4)	0(4)
N2	7(4)	11(4)	15(5)	1(4)	-1(4)	-3(4)
N5	6(4)	14(4)	13(4)	3(4)	-3(3)	-3(4)
C6	12(6)	7(5)	15(6)	-5(4)	4(4)	-1(4)
O4	34(7)	60(10)	42(8)	3(6)	19(7)	0(6)
C3	10(5)	11(5)	7(5)	3(4)	0(4)	-3(4)
C4	6(5)	13(5)	8(5)	1(4)	-3(4)	2(4)
O7	16(4)	13(4)	25(5)	8(4)	5(3)	0(3)
O8	40(7)	26(6)	37(7)	2(5)	-5(5)	-11(4)

Table S11. Selected bond lengths for $Lu(H_{1.5}C_6N_7O_3)_2 \cdot 10H_2O$.

Bond	Length (Å)	Bond	Length (Å)
Lu1-O1	2.276(10)	N1-C1	1.372(15)
Lu1-O1[1]	2.277(9)	N1-C2	1.287(14)
Lu1-O5	2.408(13)	N6-C5	1.297(18)
Lu1-O5[1]	2.408(13)	N6-C6	1.345(17)
Lu1-O6	2.382(14)	O3-C3	1.231(14)
Lu1-O6[1]	2.382(14)	N3-C5	1.348(17)
Lu1-O4[1]	2.364(16)	N3-C1	1.350(16)
Lu1-O4	2.364(16)	N7-C6	1.404(14)
N4-C5	1.401(13)	N7-C4	1.373(16)
N4-C2	1.407(14)	C2-N2	1.350(15)
N4-C4	1.356(14)	N2-C3	1.372(15)
O1-C1	1.245(16)	N5-C3	1.385(14)
O2-C6	1.242(15)	N5-C4	1.298(16)

[1]1-X,1-Y,+Z.

Table S12. Selected bond angles for $Lu(H_{1.5}C_6N_7O_3)_2 \cdot 10H_2O$.

Angle	(°)	Angle	(°)
O1-Lu1-O1[1]	137.5(6)	C5-N4-C2	118.6(10)
O1[1]-Lu1-O5[1]	127.9(4)	C4-N4-C5	122.4(10)
O1[1]-Lu1-O5	71.9(4)	C4-N4-C2	118.7(9)
O1-Lu1-O5[1]	71.9(4)	C1-O1-Lu1	149.5(9)
O1-Lu1-O5	127.9(4)	C2-N1-C1	116.7(10)
O1-Lu1-O6	139.6(4)	C5-N6-C6	119.9(10)
O1[1]-Lu1-O6	76.1(4)	C5-N3-C1	120.6(11)
O1[1]-Lu1-O6[1]	139.6(4)	C4-N7-C6	122.8(9)
O1-Lu1-O6[1]	76.1(4)	N6-C5-N4	121.3(12)
O1-Lu1-O4	74.4(5)	N6-C5-N3	121.4(10)
O1[1]-Lu1-O4	75.8(5)	N3-C5-N4	117.3(12)
O1[1]-Lu1-O4[1]	74.4(5)	O1-C1-N1	116.2(11)
O1-Lu1-O4[1]	75.8(5)	O1-C1-N2	120.5(11)
O5-Lu1-O5[1]	130.5(6)	N3-C1-N1	123.3(11)
O6-Lu1-O5[1]	68.3(4)	N1-C2-N4	123.2(10)
O6[1]-Lu1-O5	68.3(4)	N1-C2-N2	122.3(10)
O6[1]-Lu1-O5[1]	76.6(4)	N2-C2-N4	114.4(9)
O6-Lu1-O5	76.6(4)	C2-N2-C3	125.3(10)
O6[1]-Lu1-O6	88.1(7)	C4-N5-C3	116.4(10)
O4[1]-Lu1-O5	75.8(5)	O2-C6-N6	124.3(11)
O4-Lu1-O5	147.1(5)	O2-C6-N7	116.6(11)
O4-Lu1-O5[1]	75.8(5)	N6-C6-N7	119.1(10)
O4[1]-Lu1-O5[1]	147.1(5)	O3-C3-N2	119.9(12)
O4[1]-Lu1-O6	144.5(4)	O3-C3-N5	121.6(12)
O4-Lu1-O6[1]	144.5(4)	N2-C3-N5	118.5(9)
O4-Lu1-O6	101.8(5)	N4-C4-N7	114.4(10)
O4[1]-Lu1-O6[1]	101.8(5)	N5-C4-N4	126.6(11)
O4-Lu1-O4[1]	89.7(8)	N5-C4-N7	118.9(10)

[1]1-X,1-Y,+Z

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