Supporting Information

New Up-Conversion Luminescence in Molecular Cyano-substituted Naphthylsalophen Lanthanide(III) Complexes

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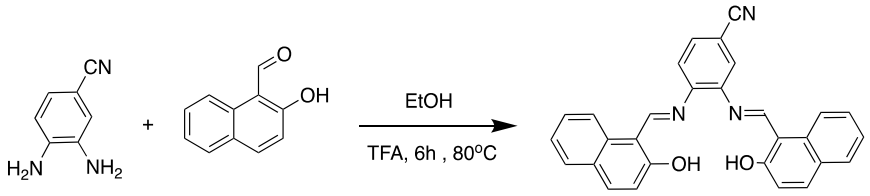
Experimental section

Unless otherwise indicated, all reactions were done open to air. Reagents were used as received. Solvents were dried by standard methods.

Purities of compounds were established via NMR and energy dispersive X-ray spectroscopy (EDS, INCA). EDS (INCA) was performed using a Zeiss EVO 50VP field emission scanning electron microscope. For both the bimetallic Yb/Er and trimetallic Y/Yb/Er samples, analysis was performed on three different regions with the same area (~300 μm × 200 μm) to obtain an average and standard deviation for elemental composition. Samples were washed with methanol then adhered with carbon tape to an aluminum stub followed by pressing the sample to the carbon tape. Excess powder was removed to ensure an evenly distributed powder coating.

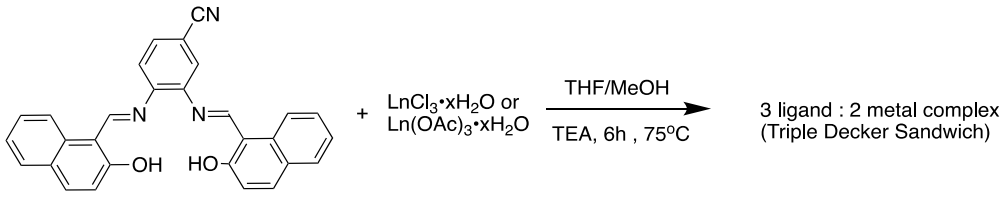
All photophysical measurements are the average of at least three independent measurements, and, unless otherwise indicated, performed at 25.0 ± 0.1°C.

Synthesis of cyano-naphthylsalophen L-CN



Aliquots of 3,4-diaminobenzonitrile (0.136 g, 1.02 mmol), TFA (162 μL, 2.11 mmol), and 2-hydroxynaphthaldehyde (0.363 g, 2.11 mmol) were added to 50 mL of EtOH in a 100ml round bottom flask, and refluxed for 6 hours. During this time, the solution changed from yellow to orange and an orange precipitate formed. The solution was allowed to cool to room temperature. The resulting solid was filtered and washed with hexanes to yield an orange powder (0.4614 g, 61 %). TOF MS (ESI) m/z $(M + H)^+$ Calc. 442.1556, Found 442.1568; ^{1}H NMR (400 MHz, DMF-d7) δ 7.07 (d, 1H, *J* = 9.2 Hz), 7.13 (d, 1H, *J* = 9.1 Hz), 7.42 (dd, 2H, *J* = 8.4, 7.3 Hz), 7.86 – 7.93 (m, 4H), 8.06 (d, 1H, *J* = 9.6 Hz), 8.12 (d, 1H, *J* = 8.3 Hz), 8.41 (s, 1H), 8.66 (dd, 2H, *J* = 12.5, 8.5 Hz), 9.87 (s, 1H), 9.96 (s, 1H), 14.97 (s, 2H). FT-IR (ATR): 2224 cm^{-1}(νC≡N),3045 cm^{-1} (νR-OH). Elemental Analysis (calcd. %) for $C_{29}H_{19}N_3O_2$: C, 78.90; H, 4.34; N, 9.52; Found: C, 78.71; H, 4.41; N, 9.67

Standard method of synthesis of the cyano-naphthylsalophen-Ln(III) metal complexes



The ligand L-CN (0.174 mmol) was dissolved in 100 mL of THF in a 250ml round bottom flask. The Ln^{III} acetate or chloride (Ln^{III} = Nd^{III}, Gd^{III}, Er^{III}, or Yb^{III}) (0.087 mmol) was dissolved in MeOH and added to the solution, followed by the addition of triethylamine (TEA) (200 μL, 1.43 mmol). The solution was refluxed for 6 hours. During this time, the color changed from light orange to either light yellow or dark orange. The excess solvent was removed under reduced pressure yielding the solid sample. The solid was recrystallized from a mixure of THF and hexanes, then filtered and washed with ethanol.

Yields:

Cyanonaphthylsalophen-Er^{III}: 79%

Cyanonaphthylsalophen-Yb^{III}: 73%

Cyanonaphthylsalophen-Nd^{III}: 74%

Cyanonaphthylsalophen-Gd^{III}: 62%

Metal complexes

- Er^{III} - (TOF MS (ESI) m/z $(M + 2H)^+$ Calc. 1652.2646, Found 1652.2726.)
  - Elemental Analysis as $C_{87}H_{51}N_9O_6Er_2 \cdot 10\ H_2O$ Calc'd(%): C, 57.01; H, 3.90; N, 6.88; Found: C, 57.04; H, 4.18; N,6.76.
  - Figures S4 and S5
- Yb^{III} - (TOF MS (ESI) m/z $(M + H)^+$ Calc. 1665.2767, Found 1665.2777.)
  - Elemental Analysis as $C_{87}H_{51}N_9O_6Yb_2 \cdot 2\ H_2O$ Calc'd(%): C, 61.45; H, 3.26; N, 7.41; Found: C, 61.67; H, 3.71; N, 7.67.
  - Figures S6 and S7
- Nd^{III}- (TOF MS (ESI) m/z $(M + H)^+$ Calc. 1606.9060, Found 1606.2124.)
  - Figures S8 and S9
- Gd^{III}- (TOF MS (ESI) m/z $(M + H)^+$ Calc. 1634.2444, Found 1634.2382.)
  - Figure S10 and S11

The mixed Ln^{III} complexes ($[Yb_{0.86}Er_{0.14})_2(L\text{-}CN)_3]$ and $[Y_{0.76}Yb_{0.16}Er_{0.08})_2(L\text{-}CN)_3]$) were synthesized adapting the procedure described for the homonuclear complexes synthesis. CN-L (0.0601 mmol, 0.0265g) was dissolved in a 100mL of THF, and 3 equivalents of TEA (0.1801 mmol, 26 μL) were added to fully deprotonate the ligand. Ln^{III} chloride solutions, in MeOH (15 mL), containing a mixture of Yb^{III} and Er^{III} (Yb: 0.0344 mmol, 0.0156g; Er: 0.0056, 0.0021g) or Y^{III}, Yb^{III} and Er^{III} (Y: 0.0280mmol, 0.0085g; Yb: 0.0100 mmol, 0.0039g; Er: 0.002 mmol, 0.0002g) were added to the solution of the deprotonated ligand in 2:3 (Ln:L) molar ratio, and kept under stirring for 6 h at 75 ºC to produce a bright red-brownish precipitate. The precipitate was filtered, washed with cold water, and dried under reduced pressure to yield the desired complexes. Percentages of metal content were calculated in each case by taking the total molar concentration of metal required to keep the 3 Lig: 2 M ratio and multiplying it by the percentage of metal desired in each species.

$[Yb_{0.78}Er_{0.22})_2(L\text{-}CN)_3]$ – ESI-MS m/z $(M + H)^+$ calc. , found , Figure S12; EDS was taken from multiple spots on sample for statistical analysis; EDS (78.11±1.56) at.% Yb, (21.89±1.56) at.% Er

CN-Yb*Er	Yb (atomic%)	Er (atomic%)
1	78.04	21.96
2	76.78	23.22
3	80.5	19.5
4	76.66	23.34
5	78.55	21.45
Avg	78.106	21.894
Std Dev	1.563803057	1.563803057

$[Y_{0.76}Yb_{0.16}Er_{0.08})_2(L\text{-}CN)_3]$ –EDS was taken from multiple spots on sample for statistical analysis; EDS (75.83±1.55) at.% Y, (16.38±1.31) at.% Yb, (7.79±0.74) at.% Er

CN-Y*Yb*Er	Y (atomic%)	Yb (atomic%)	Er (atomic%)
1	76.64	16.04	7.33
2	75.43	17.45	7.12
3	77.4	14.67	7.94
4	73.86	17.36	8.78
Avg	75.8325	16.38	7.7925
Std Dev	1.545086297	1.309580085	0.744552438

Photophysical characterization. Solutions of the metal complex ($1x10^{-4}$ M) in dichloromethane were used to obtain both the emission and excitation spectra. The photoluminescence data were obtained using a Fluorolog-3 spectrofluorimeter (Horiba FL3-22-iHR550), with 1200 grooves/mm excitation monochromator gratings blazed at 330 nm and 1200 grooves/mm or 600 grooves/mm emission monochromator gratings blazed at 500 nm or 1000 nm for UV-Vis or NIR range, respectively. A 450 W ozone-free xenon lamp (Ushio) was used as the radiation source. The excitation spectra, corrected for instrumental function, were measured between 250 and 600 nm. The emission spectra were measured in the range 350-800 nm using a Hamamatsu 928P and in the range 1220-1320 nm using a Hamamatsu 5509-73 cooled with liquid N_2. All emission spectra were corrected for instrumental function. The emission decay curves were obtained using a TCSPC system and a Horiba SpectraLED model S-370 (peak wavelength = 370 ± 10 nm, ~4 pJ/pulse) as excitation source. Before all decay curves measurements, a blank was obtained using Ludox®. The energies of the ligand's singlet and triplet levels were obtained at ~77 K by deconvolution of

the fluorescence and phosphorescence spectra, respectively, into their Franck-Condon progression and are reported as the 0-0 transition.[1] The quantum yield of the samples was determined by the dilution method using Equation 1. The standard for quantum yield measurements was $[Yb(tta)_3(H_2O)_2]$ ($\phi \sim 0.12\%$, $1x10^{-4}$ M in toluene).[2] The excitation wavelength for both sample and quantum yield standard was chosen to ensure a linear relationship between the intensity of emitted light and the concentration of the absorbing/emitting species ($A \leq 0.05$).

$$\Phi_x = \frac{Grad_x}{Grad_{std}} \times \frac{n_x^2}{n_{std}^2} \times \frac{I_{std}}{I_x} \Phi_{std} \qquad (1)$$

Grad is the slope of the plot of the emission area as a function of the absorbance, *n* is the refractive index of the solvent, *I* is the intensity of the excitation source at the excitation wavelength and Φ is the quantum yield for sample *x* and standard *std*.

The upconversion emission spectra were obtained using a 980 nm laser operating in continuous wave mode (beam diameter 5 x 8 mm^2, Opto Engine MDL-III-980nm-2.5W).

^{1}H NMR spectroscopy

^{1}H NMR were recorded on a Bruker AV 600 MHz spectrometer using DMF-d7 (Cambridge Isotope Laboratories). Chemical shifts are reported in parts per million (δ) and are referenced against residual internal solvent signals.

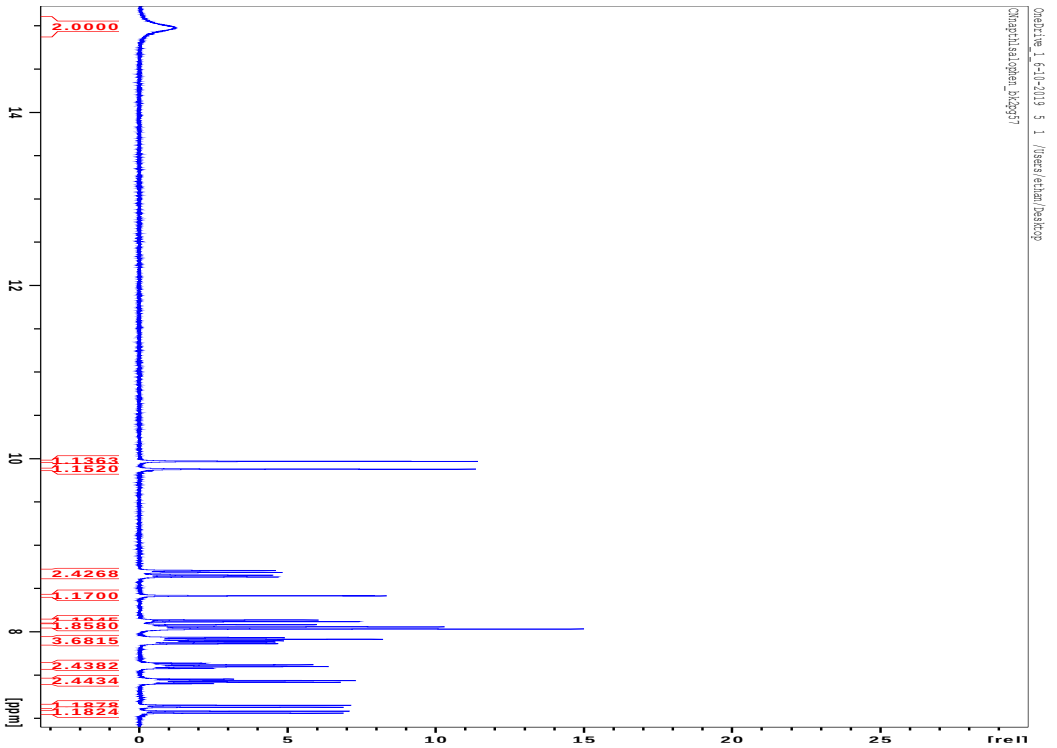


Figure S1. ^{1}H NMR spectrum of cyano-naphthylsalophen H_2L-CN.

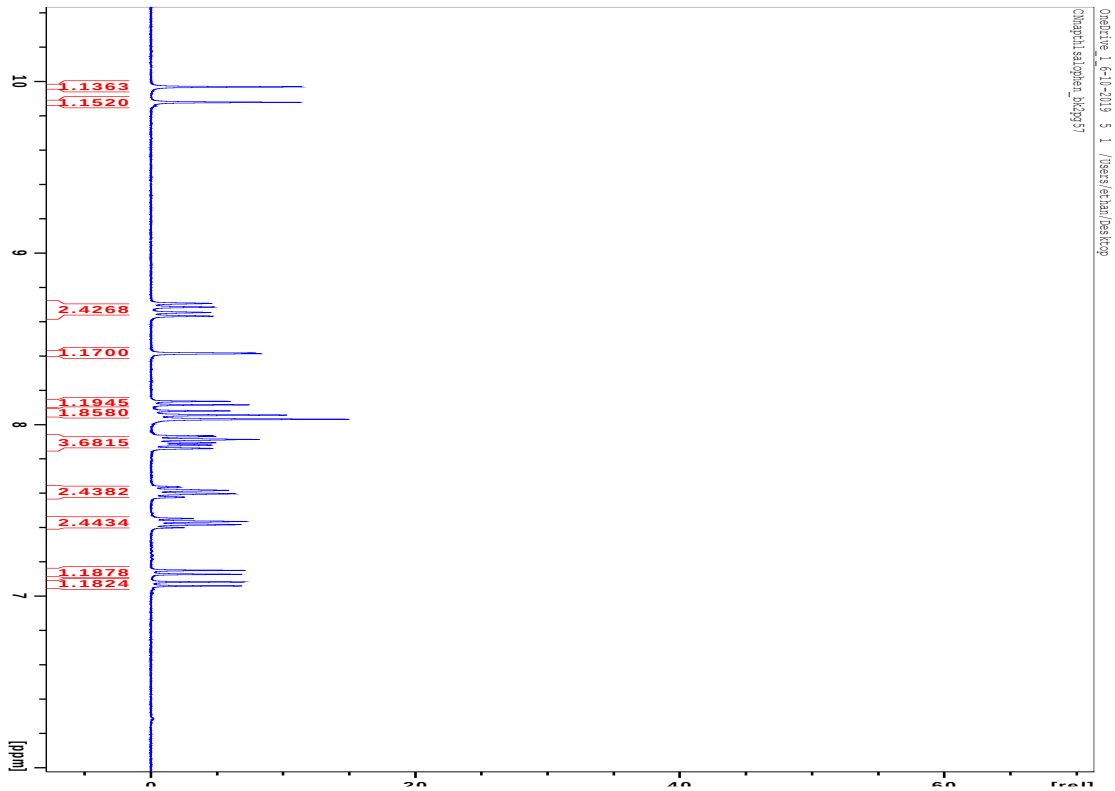


Figure S2. Aromatic region of the ^{1}H NMR spectrum of cyano-naphthylsalophen H_2L-CN.

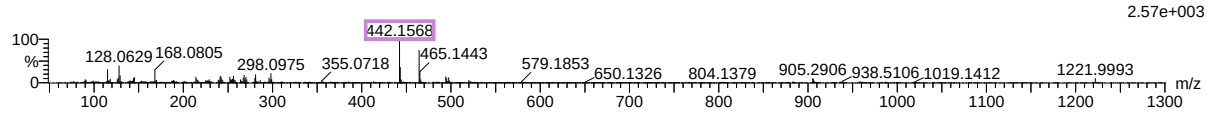
Mass spectrometry

Analysis was performed using a syringe pump with a syringe filled with acetonitrile or sample diluted in acetonitrile at flow rate of 2 to 10 µL/min into a quadrupole time-of-flight mass spectrometer (Q-Tof Premier, Waters) with electrospray ionization (ESI) in positive mode. Data were collected and processed with Masslynx software (V4.1). The capillary voltage was set at 3.1 kV, the sample cone voltage was 30 V, and the extraction cone was 4.3 V. The source and desolvation temperature were maintained at 105 and 300 °C, respectively, with the desolvation gas flow set at 500 L/h. The Time of Flight mass spectrometer scan was 1 s long from 50 to 3000 m/z with a 0.1 s inter-scan delay in the centroid data format. A lock mass was used to correct instrument accuracy with a 0.1 µM solution of HP 1221 (Agilent part number G1969-85003).

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-50 N: 0-3 O: 0-2
EH_AG_JPG29ACNLigand 15 (0.314) Cm (15:16)
1: TOF MS ES+



Minimum:				-1.5			
Maximum:		5000.0	20.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
442.1568	442.1556	1.2	2.7	21.5	199.6	0.0	C29 H20 N3 O2

Figure S3. Mass spectrum of cyano-naphthylsalophen L-CN.

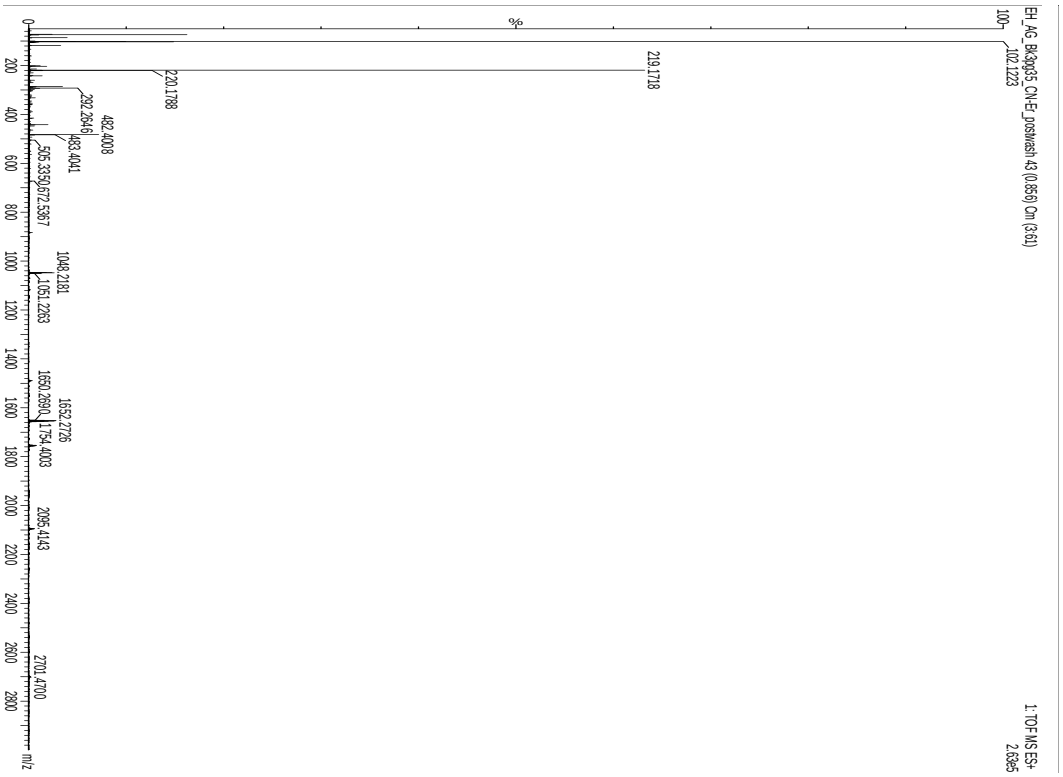


Figure S4. Mass spectrum of the cyano-naphthylsalophen-Er^{III} complex.

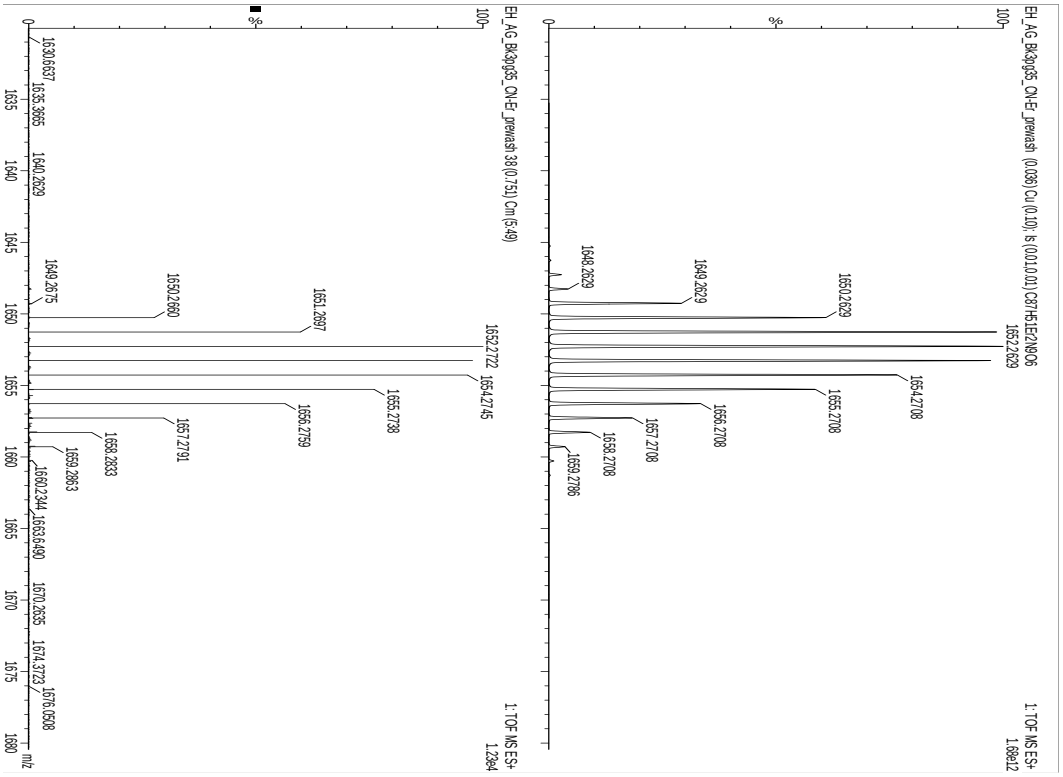


Figure S5. Isotopic distribution pattern of the molecular ion peak of the cyano-naphthylsalophen-Er^{III} complex. Top: calculated, bottom: experimental.

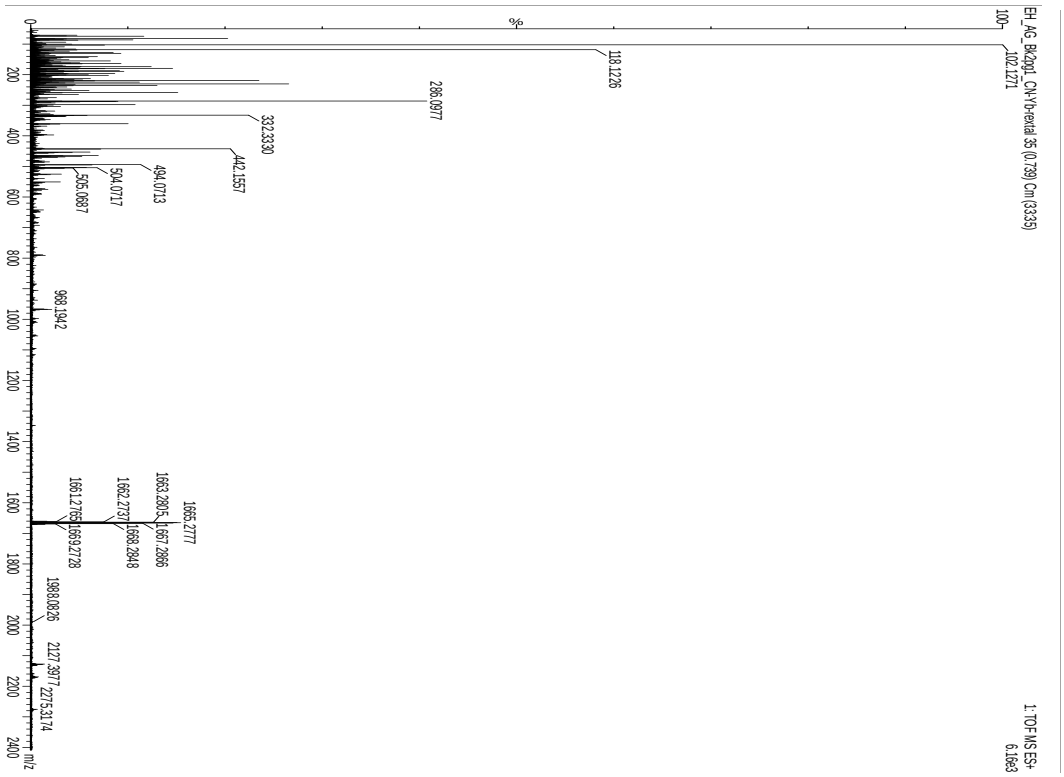


Figure S6. Mass spectrum of the Yb^{III} complex of cyano-naphthylsalophen.

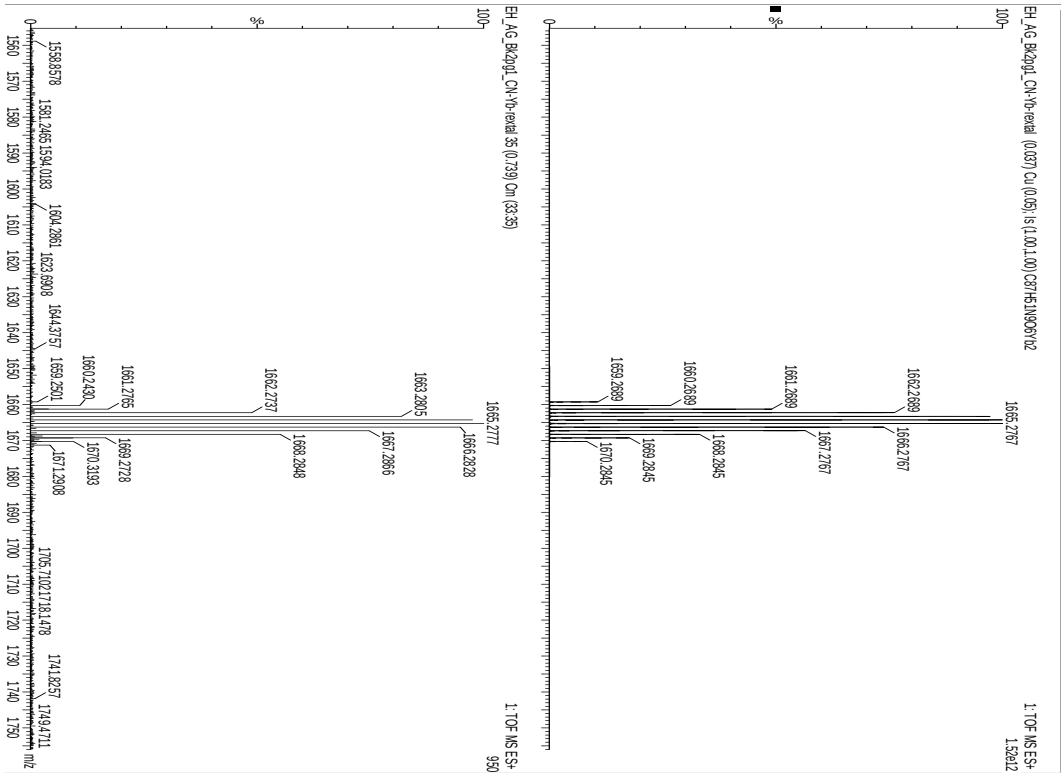


Figure S7. Isotope distribution pattern of the molecular ion peak of the cyano-naphthylsalophen-Yb^{III} complex. Top: calculated, bottom: experimental.

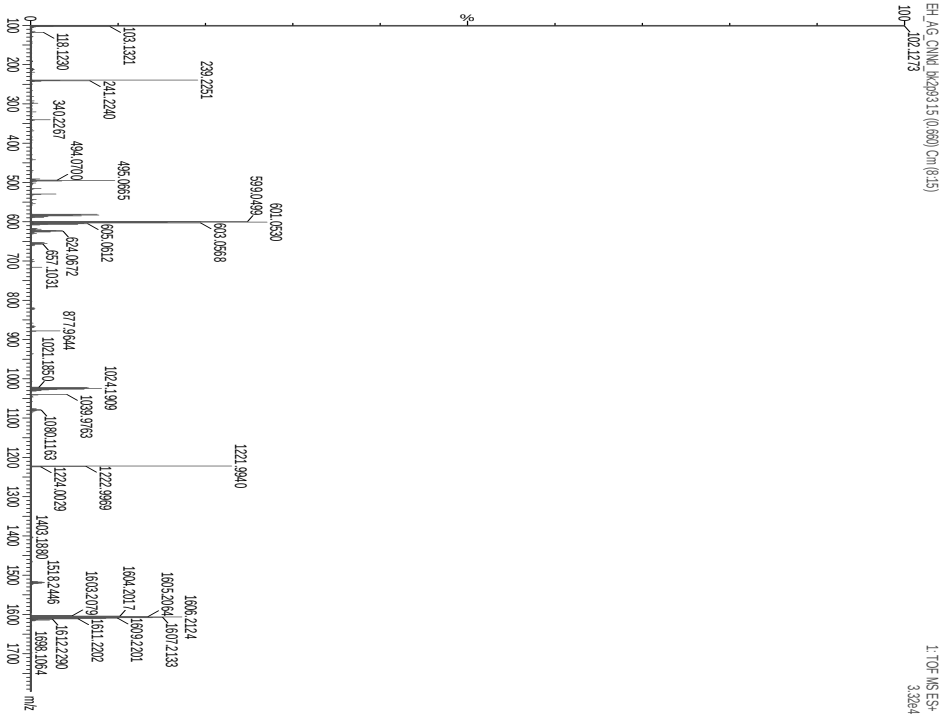


Figure S8. Mass spectrum of the Nd^{III} complex of cyano-naphthylsalophen.

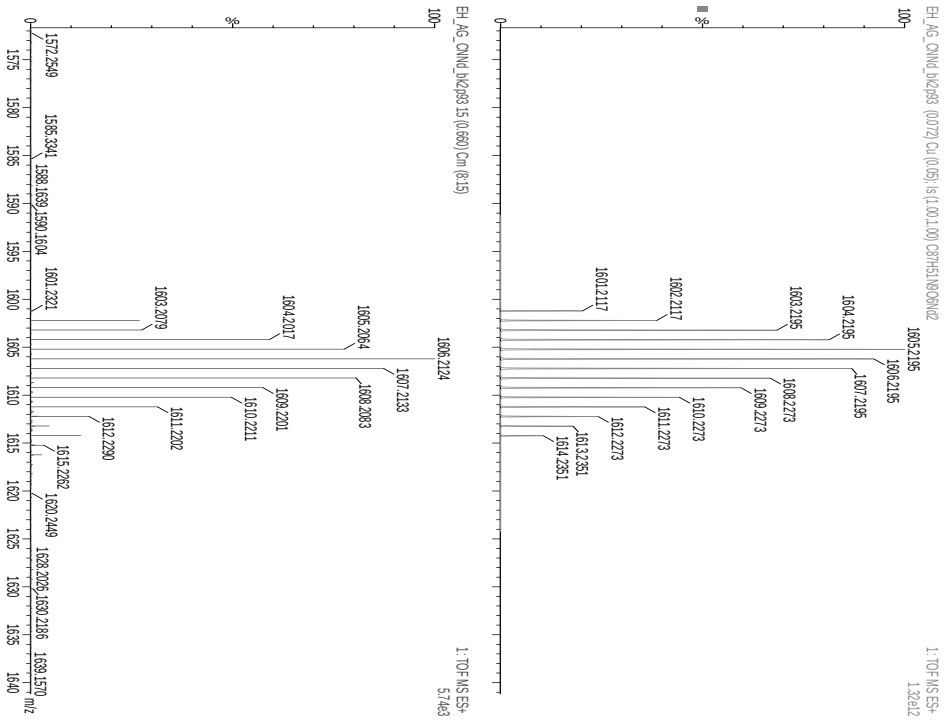


Figure S9. Isotope distribution pattern of the molecular ion peak of the cyano-naphthylsalophen-Nd^{III} complex. Top: calculated, bottom: experimental.

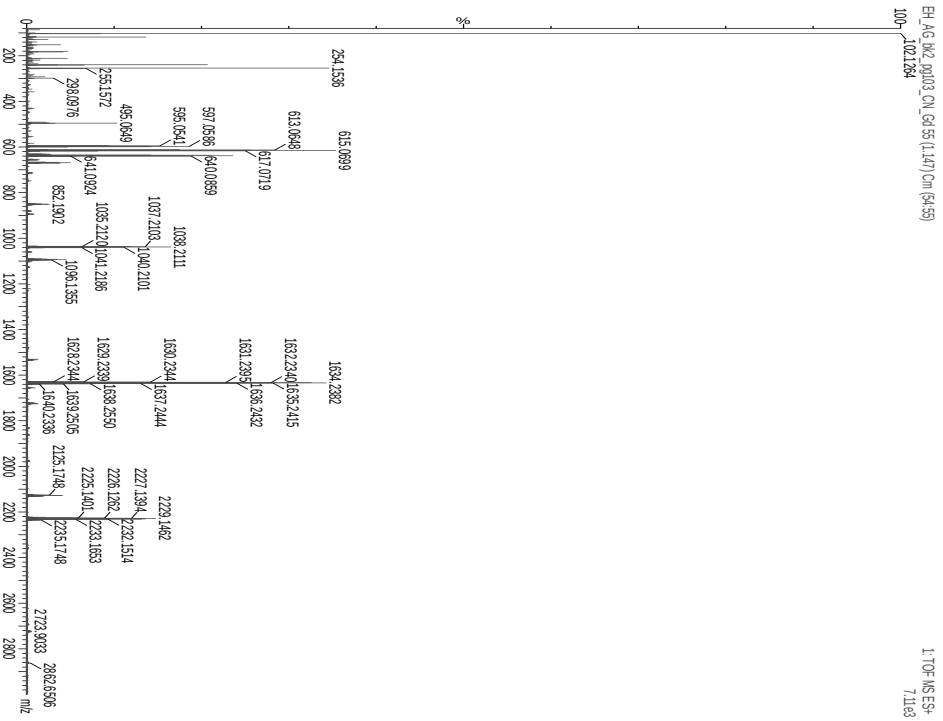


Figure S10. Mass spectrum of the Gd^{III} complex of cyano-naphthylsalophen.

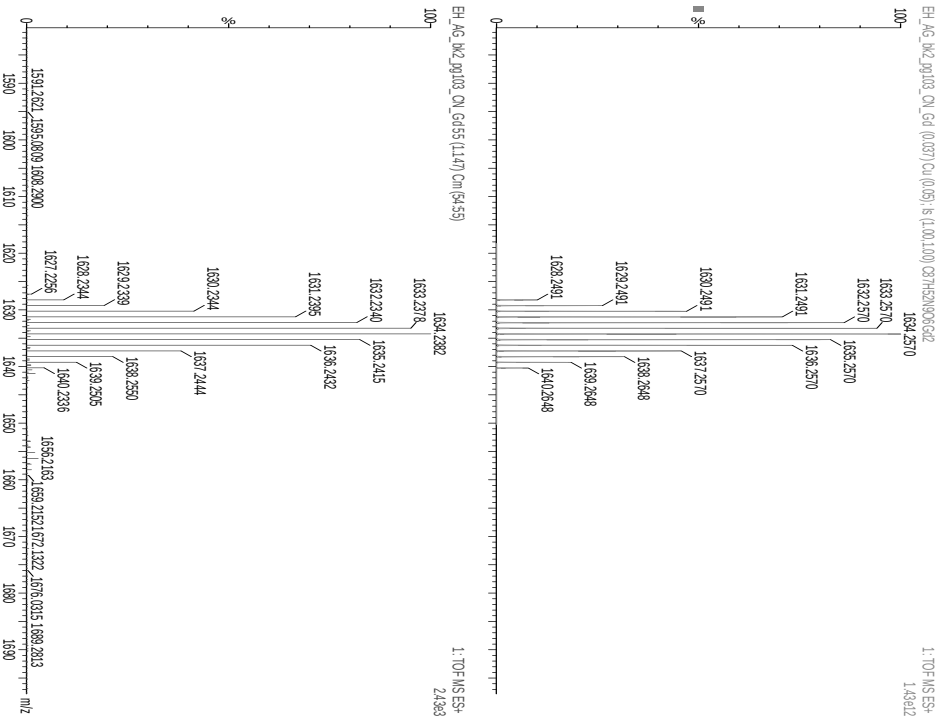


Figure S11. Isotope distribution pattern of the molecular ion peak of the cyano-naphthylsalophen-Gd^{III} complex. Top: calculated, bottom: experimental.

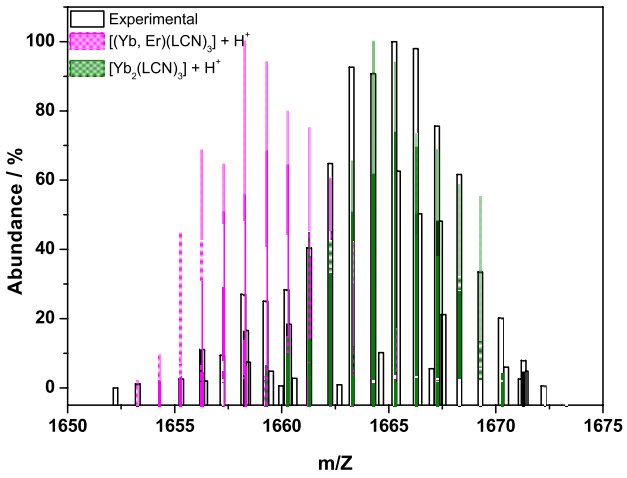


Figure S12. ESI-MS of a) $[(Yb_{0.86}Er_{0.14})_2(L\text{-}CN)_3]$ (black line), and isotope patterns ($[(Yb_{0.5}Er_{0.5})_2(L\text{-}CN)_3]$ – pink line, $[Yb_2(L\text{-}CN)_3]$ – green line).

FT-IR spectroscopy

Infrared spectra were obtained in the solid state using an attenuated total reflectance (ATR) method on a Thermo Scientific Nicolet iS50 FT-IR instrument.

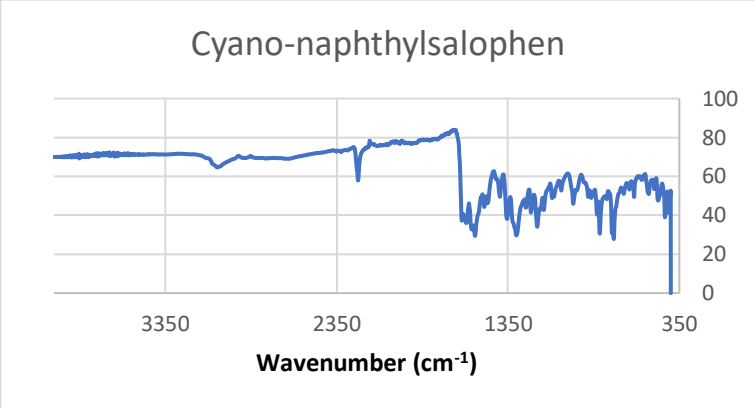


Figure S13. IR spectrum of cyano-naphthylsalophen $H_2L\text{-}CN$.

Photophysical characterization

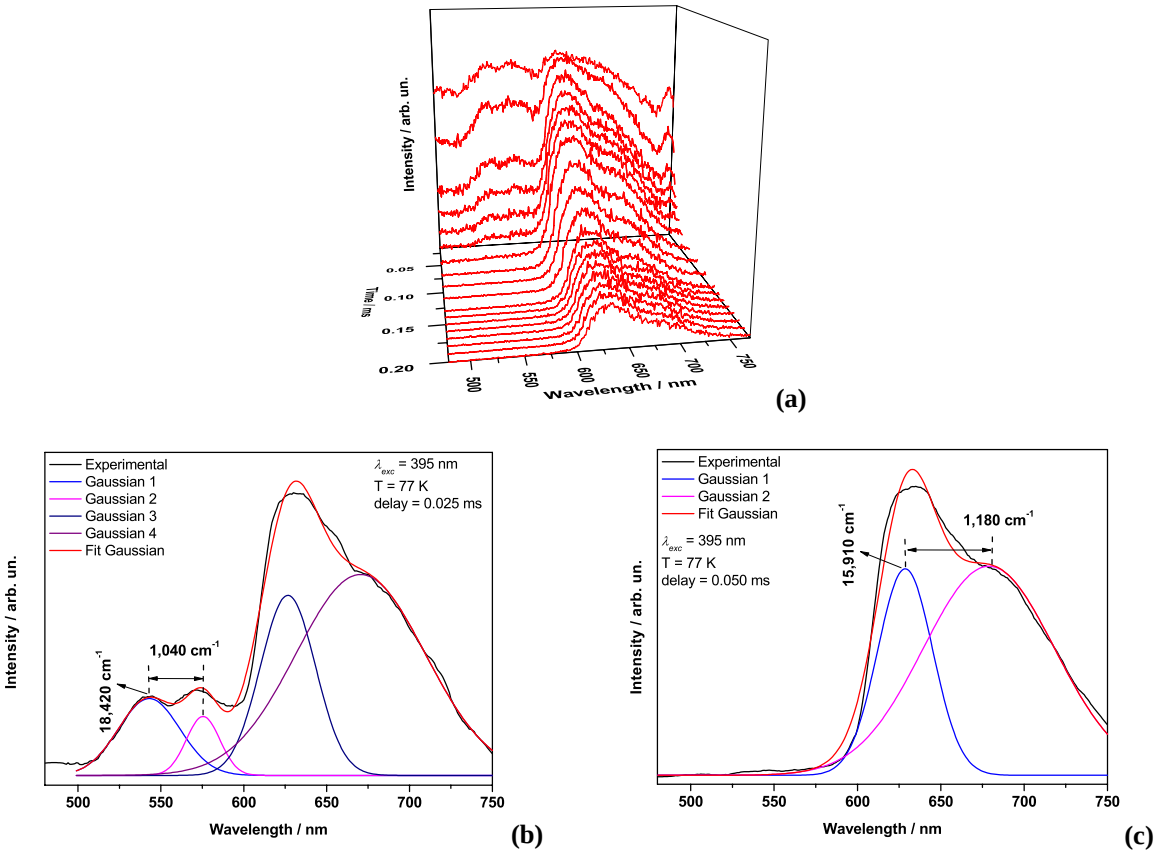


Figure S14. (a) Time-resolved emission spectra of $[Gd_2(L\text{-}CN)_3]$. Deconvolution of the (b) fluorescence and (c) phosphorescence emission bands. [complex] = $1x10^{-4}$ M in dichloromethane, T = 77 K and λ_{exc} = 395 nm.

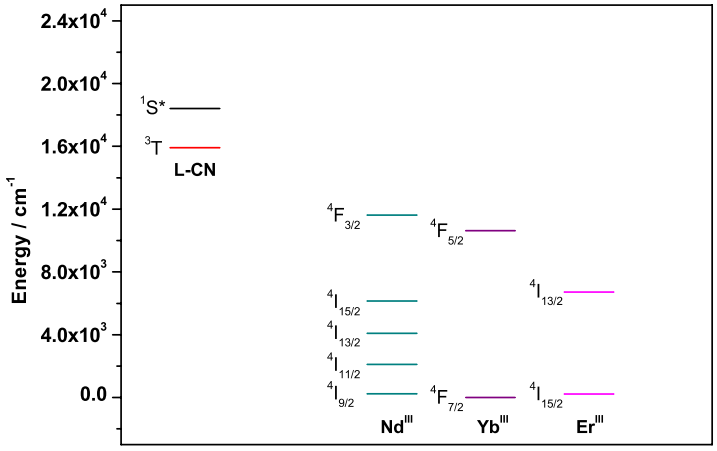


Figure S15. Energy level diagram with the singlet and triplet levels of the ligand and the electronic levels of Nd^{III}, Yb^{III} and Er^{III}.

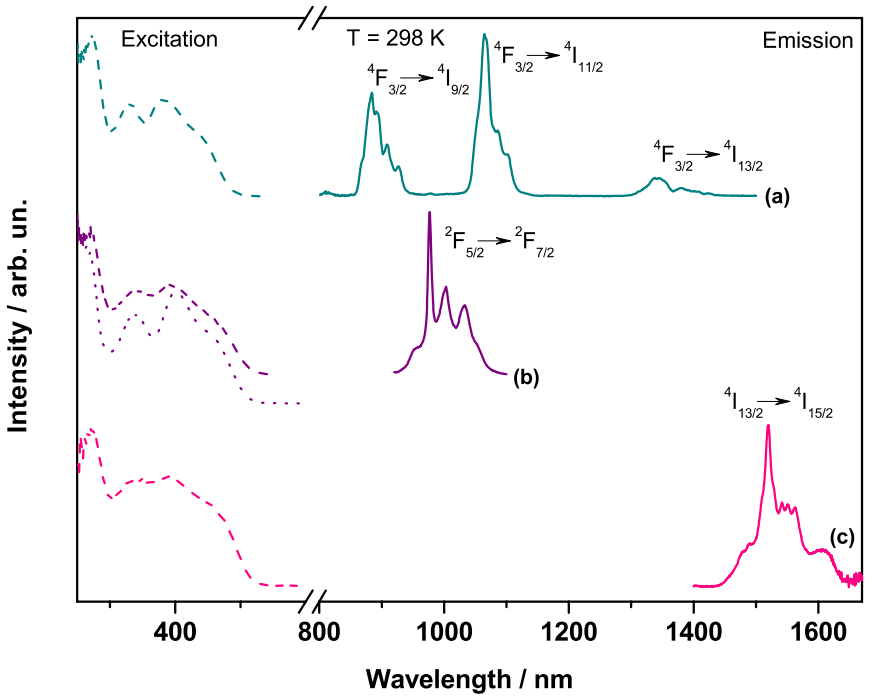
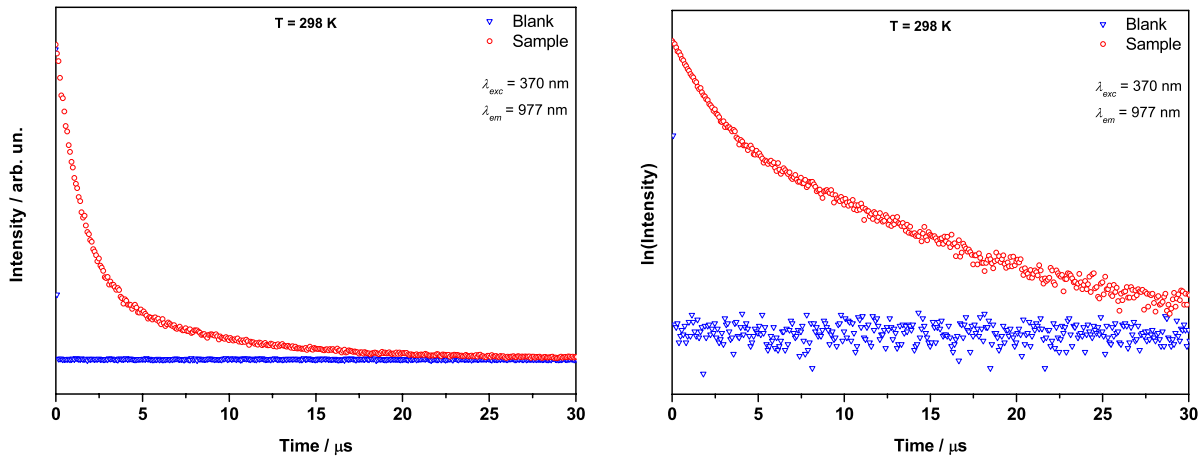


Figure S16. One-photon excitation (dashed lines, left) and emission spectra (solid lines, right) of (a) Nd^{III} (green), (b) Yb^{III} (purple) and (c) Er^{III} (pink) complexes. λ_{exc} = 380 nm, [complex] = 1×10^{-4} M in CH_2Cl_2 and T = 298 K. The absorption spectrum (dotted purple line, left) of the Yb^{III} complex is shown for comparison.



(a) **(b)**

Figure S17. Emission lifetime decay curves of the complex $[Yb_2(L\text{-}CN)_3]$ obtained in CH_2Cl_2 at 298 K. (a) Exponential decay. (b) Linearization.

Table S1. Slopes for the plots of log(I) as a function of log(P) and corresponding values of R^2.

Transition	Slope	R^2
$^4S_{3/2} \rightarrow {}^4I_{15/2}$	1.70 ± 0.05	0.982
$^4I_{9/2} \rightarrow {}^4I_{15/2}$	2.06 ± 0.26	0.984

Crystallographic characterization

Crystals suitable for single crystal X-ray diffraction were selected and mounted on a 50-micron MiTeGen loop using Paratone-N oil and data set collection was completed on a Bruker D8 VENTURE κ-geometry diffractometer using Cu Kα radiation (Incoatec IμS DIAMOND microfocus sealed tube (λ = 1.54178 Å). Crystals were kept at 100 K during unit cell and data collection. Determination of the unit cell and collection of data were performed using the APEX III software, and determination of integrated intensities and global cell refinement were performed with the Bruker SAINT software package. An empirical absorption correction (SADABS) was applied. Structures were solved using Intrinsic Phasing/Direct Methods.[3, 4] (ShelXT) and least-squares refinement was performed using ShelXL in APEX III. Projections were created on Olex2.1.

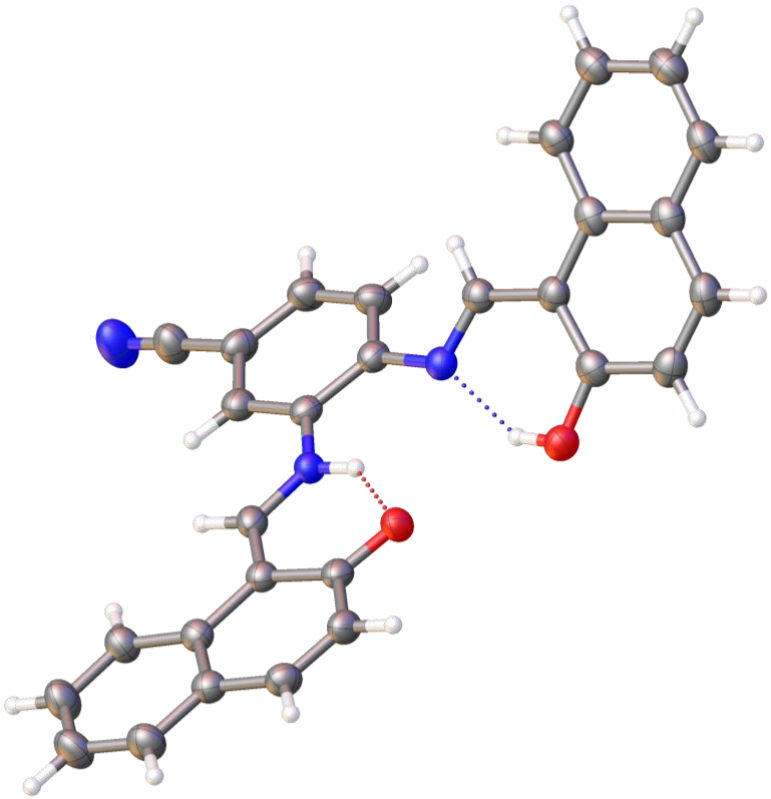


Figure S18. Projection of front view of L-CN. Carbon atoms are shown in grey, nitrogen in blue, and oxygen in red. Intramolecular hydrogen-bonding interactions are shown as dashed lines.

Table S2. Sample and crystal data for L-CN.

Identification code	Ethan102519	
CCDC	1964321	
Chemical formula	$C_{29}H_{19}N_3O_2$	
Formula weight	441.47 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 A	
Crystal size	0.008 × 0.035 × 0.153 mm	
Crystal habit	clear pale orange thin rod	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 10.8315(7)Å	α = 90°
	b = 7.1085(4)Å	β = 90.302(4)°
	c = 27.6783(18)Å	γ = 90°
Volume	2131.1(2) A3	
z	4	
Density (calculated)	1.376 g/cm^3	

Absorption coefficient	0.703 mm^{-I}
F(000)	920

Table S3. Data collection and structure refinement for L-CN.

Diffractometer	Bruker D8 VENTURE K-geometry diffractometer
Radiation source	Incoatec IμS DIAMOND microfocus sealed tube (Cu Ku, ').,, = 1.54178 Å)
Theta range for data collection Index ranges	3.19 to 72.11°
Index ranges	-13<=h<=13, -8<=k<=7, -34<=1<=34
Reflections collected	31468
Independent reflections	4186 [R(int) = 0.0932]
Coverage of independent reflections	99.9%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9940 and 0.9000
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma w(F_0^2 - F_c^2)^2$
Data / restraints / parameters	4186 / 0 / 308
Goodness-of-fit on F2	1.051
Final R indices	2754 data; 1>2cr(I) R1 = 0.0609, wR2 = 0.1570
	all data. R1 = 0.0949, wR2 = 0.1780
Weighting scheme	$w=l/[\ \sigma^2(F_0^2)+(0.0723P)^2+ 1.4534P]$ where $P=(F_0^2+2F_c^2)/3$
Largest diff. peak and hole	0.482 and -0.237 $eÅ^{-3}$
R.M.S. deviation from mean	0.053 $eÅ^{-3}$

Table S4. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for L-CN.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
O001	0.76327(16)	0.6622(3)	0.26372(6)	0.0371(5)
O002	0.59230(17)	0.4377(3)	0.19197(6)	0.0384(5)
N003	0.62965(18)	0.5917(3)	0.33690(7)	0.0294(5)
N004	0.45709(19)	0.5017(3)	0.26819(7)	0.0313(5)
C005	0.8350(2)	0.7088(4)	0.34459(9)	0.0300(6)
C006	0.7239(2)	0.6468(4)	0.36388(9)	0.0313(6)
C007	0.5145(2)	0.5274(4)	0.35248(9)	0.0299(6)

	x/a	y/b	z/c	U(eq)
C008	0.4254(2)	0.4820(4)	0.31723(9)	0.0317(6)
C009	0.8484(2)	0.7162(4)	0.29272(9)	0.0315(6)
C00A	0.4963(2)	0.5013(4)	0.16567(9)	0.0345(6)
C00B	0.3721(2)	0.5599(4)	0.23840(9)	0.0321(6)
C00C	0.0462(2)	0.8391(4)	0.35389(9)	0.0335(6)
C00D	0.3058(3)	0.6346(4)	0.10464(10)	0.0363(6)
C00E	0.3879(2)	0.5683(4)	0.18659(9)	0.0325(6)
C00F	0.4851(2)	0.5084(4)	0.40109(9)	0.0342(6)
C00G	0.9373(2)	0.7686(4)	0.37550(9)	0.0310(6)
C00H	0.2898(2)	0.6381(4)	0.15570(9)	0.0338(6)
C00I	0.3105(2)	0.4127(4)	0.33163(10)	0.0360(6)
C00J	0.1777(2)	0.7105(4)	0.17323(9)	0.0355(6)
C00K	0.9612(2)	0.7916(4)	0.27354(9)	0.0361(6)
C00L	0.0537(2)	0.8497(4)	0.30235(9)	0.0364(6)
C00M	0.5086(3)	0.4944(4)	0.11497(10)	0.0381(7)
C00N	0.9341(3)	0.7598(4)	0.42647(9)	0.0374(6)
C00O	0.2813(3)	0.3929(4)	0.37963(10)	0.0383(6)
C00P	0.3682(3)	0.4414(4)	0.41427(9)	0.0378(7)
N00Q	0.3211(2)	0.3863(5)	0.50481(9)	0.0606(8)
C00R	0.2119(3)	0.7050(4)	0.07438(10)	0.0412(7)
C00S	0.4168(3)	0.5588(4)	0.08562(10)	0.0411(7)
C00T	0.1041(3)	0.7740(4)	0.09244(10)	0.0436(7)
C00U	0.0871(3)	0.7759(4)	0.14238(10)	0.0397(7)
C00V	0.1445(3)	0.9022(4)	0.38297(10)	0.0427(7)
C00W	0.0324(3)	0.8210(5)	0.45404(10)	0.0453(7)
C00X	0.3409(3)	0.4124(5)	0.46444(10)	0.0440(7)
C00Y	0.1379(3)	0.8945(5)	0.43251(11)	0.0470(8)

Table S5. Bond lengths (Å) for L-CN.

O001-C009	1.278(3)	O002-C00A	1.344(3)
O002-H002	0.84	N003-C006	1.321(3)
N003-C007	1.398(3)	N003-H003	0.88
N004-C00B	1.300(3)	N004-C008	1.409(3)
C005-C006	1.390(4)	C005-C009	1.445(3)
C005-C00G	1.460(4)	C006-H006	0.95
C007-C00F	1.391(3)	C007-C008	1.407(4)
C008-C00I	1.398(4)	C009-C00K	1.439(4)

C00A-C00E	1.396(4)	C00A-C00M	1.411(4)
C00B-C00E	1.446(3)	C00B-H00B	0.95
C00C-C00V	1.406(4)	C00C-C00G	1.417(4)
C00C-C00L	1.431(4)	C00D-C00R	1.406(4)
C00D-C00S	1.421(4)	C00D-C00H	1.425(4)
C00E-C00H	1.449(4)	C00F-C00P	1.403(4)
C00F-H00F	0.95	C00G-C00N	1.413(3)
C00H-C00J	1.407(4)	C00I-C00O	1.375(4)
C00I-H00I	0.95	C00J-C00U	1.378(4)
C00J-H00J	0.95	C00K-C00L	1.342(4)
C00K-H00K	0.95	C00L-H00L	0.95
C00M-C00S	1.360(4)	C00M-H00M	0.95
C00N-C00W	1.378(4)	C00N-H00N	0.95
C00O-C00P	1.384(4)	C00O-H00O	0.95
C00P-C00X	1.436(4)	N00Q-C00X	1.154(4)
C00R-C00T	1.364(4)	C00R-H00R	0.95
C00S-H00S	0.95	C00T-C00U	1.396(4)
C00T-H00T	0.95	C00U-H00U	0.95
C00V-C00Y	1.375(4)	C00V-H00V	0.95
C00W-C00Y	1.393(4)	C00W-H00W	0.95
C00Y-H00Y	0.95		

Table S6. Bond angles (°) for L-CN.

C00A-O002-H002	109.5	C006-N003-C007	127.6(2)
C006-N003-H003	116.2	C007-N003-H003	116.2
C00B-N004-C008	117.9(2)	C006-C005-C009	119.0(2)
C006-C005-C00G	121.5(2)	C009-C005-C00G	119.4(2)
N003-C006-C005	123.0(2)	N003-C006-H006	118.5
C005-C006-H006	118.5	C00F-C007-N003	122.6(2)
C00F-C007-C008	119.2(2)	N003-C007-C008	118.1(2)
C00I-C008-C007	119.5(2)	C00I-C008-N004	122.1(2)
C007-C008-N004	118.4(2)	O001-C009-C00K	119.4(2)
O001-C009-C005	122.5(2)	C00K-C009-C005	118.1(2)
O002-C00A-C00E	122.7(2)	O002-C00A-C00M	116.8(2)
C00E-C00A-C00M	120.5(2)	N004-C00B-C00E	123.7(2)
N004-C00B-H00B	118.1	C00E-C00B-H00B	118.1
C00V-C00C-C00G	120.1(2)	C00V-C00C-C00L	120.5(2)

C00G-C00C-C00L	119.4(2)	C00R-C00D-C00S	121.7(2)
C00R-C00D-C00H	119.6(3)	C00S-C00D-C00H	118.8(3)
C00A-C00E-C00B	120.1(2)	C00A-C00E-C00H	119.2(2)
C00B-C00E-C00H	120.6(2)	C007-C00F-C00P	119.8(2)
C007-C00F-H00F	120.1	C00P-C00F-H00F	120.1
C00N-C00G-C00C	117.5(2)	C00N-C00G-C005	123.4(2)
C00C-C00G-C005	119.1(2)	C00J-C00H-C00D	117.3(2)
C00J-C00H-C00E	123.6(2)	C00D-C00H-C00E	119.1(2)
C00O-C00I-C008	121.4(2)	C00O-C00I-H00I	119.3
C008-C00I-H00I	119.3	C00U-C00J-C00H	121.5(2)
C00U-C00J-H00J	119.2	C00H-C00J-H00J	119.2
C00L-C00K-C009	121.9(2)	C00L-C00K-H00K	119.1
C009-C00K-H00K	119.1	C00K-C00L-C00C	122.0(2)
C00K-C00L-H00L	119.0	C00C-C00L-H00L	119.0
C00S-C00M-C00A	120.6(3)	C00S-C00M-H00M	119.7
C00A-C00M-H00M	119.7	C00W-C00N-C00G	121.1(3)
C00W-C00N-H00N	119.5	C00G-C00N-H00N	119.5
C00I-C00O-C00P	119.0(3)	C00I-C00O-H00O	120.5
C00P-C00O-H00O	120.5	C00O-C00P-C00F	121.1(2)
C00O-C00P-C00X	119.4(3)	C00F-C00P-C00X	119.4(2)
C00T-C00R-C00D	121.8(3)	C00T-C00R-H00R	119.1
C00D-C00R-H00R	119.1	C00M-C00S-C00D	121.6(3)
C00M-C00S-H00S	119.2	C00D-C00S-H00S	119.2
C00R-C00T-C00U	119.0(3)	C00R-C00T-H00T	120.5
C00U-C00T-H00T	120.5	C00J-C00U-C00T	120.8(3)
C00J-C00U-H00U	119.6	C00T-C00U-H00U	119.6
C00Y-C00V-C00C	121.0(3)	C00Y-C00V-H00V	119.5
C00C-C00V-H00V	119.5	C00N-C00W-C00Y	121.0(3)
C00N-C00W-H00W	119.5	C00Y-C00W-H00W	119.5
N00Q-C00X-C00P	178.4(4)	C00V-C00Y-C00W	119.3(3)
C00V-C00Y-H00Y	120.4	C00W-C00Y-H00Y	120.4

Table S7. Torsion angles (°) for L-CN.

C007-N003-C006-C005	-179.9(3)	C009-C005-C006-N003	0.9(4)
C00G-C005-C006-N003	-179.9(2)	C006-N003-C007-C00F	-1.8(4)
C006-N003-C007-C008	177.7(3)	C00F-C007-C008-C00I	-2.1(4)
N003-C007-C008-C00I	178.3(2)	C00F-C007-C008-N004	-179.8(2)

N003-C007-C008-N004	0.6(4)	C00B-N004-C008-C00I	38.8(4)
C00B-N004-C008-C007	-143.6(3)	C006-C005-C009-O001	-2.3(4)
C00G-C005-C009-O001	178.5(2)	C006-C005-C009-C00K	176.2(2)
C00G-C005-C009-C00K	-3.0(4)	C008-N004-C00B-C00E	-173.5(2)
O002-C00A-C00E-C00B	-4.1(4)	C00M-C00A-C00E-C00B	174.8(2)
O002-C00A-C00E-C00H	178.7(2)	C00M-C00A-C00E-C00H	-2.5(4)
N004-C00B-C00E-C00A	4.0(4)	N004-C00B-C00E-C00H	-178.8(3)
N003-C007-C00F-C00P	-179.4(2)	C008-C007-C00F-C00P	1.1(4)
C00V-C00C-C00G-C00N	-1.8(4)	C00L-C00C-C00G-C00N	179.7(3)
C00V-C00C-C00G-C005	178.3(3)	C00L-C00C-C00G-C005	-0.2(4)
C006-C005-C00G-C00N	3.2(4)	C009-C005-C00G-C00N	-177.6(3)
C006-C005-C00G-C00C	-176.9(3)	C009-C005-C00G-C00C	2.3(4)
C00R-C00D-C00H-C00J	1.0(4)	C00S-C00D-C00H-C00J	-178.7(3)
C00R-C00D-C00H-C00E	-178.9(3)	C00S-C00D-C00H-C00E	1.3(4)
C00A-C00E-C00H-C00J	-179.3(3)	C00B-C00E-C00H-C00J	3.5(4)
C00A-C00E-C00H-C00D	0.7(4)	C00B-C00E-C00H-C00D	-176.5(2)
C007-C008-C00I-C00O	1.9(4)	N004-C008-C00I-C00O	179.5(3)
C00D-C00H-C00J-C00U	-0.2(4)	C00E-C00H-C00J-C00U	179.8(3)
O001-C009-C00K-C00L	-179.8(3)	C005-C009-C00K-C00L	1.7(4)
C009-C00K-C00L-C00C	0.4(4)	C00V-C00C-C00L-C00K	-179.7(3)
C00G-C00C-C00L-C00K	-1.2(4)	O002-C00A-C00M-C00S	-178.9(3)
C00E-C00A-C00M-C00S	2.2(4)	C00C-C00G-C00N-C00W	1.2(4)
C005-C00G-C00N-C00W	-178.9(3)	C008-C00I-C00O-C00P	-0.6(4)
C00I-C00O-C00P-C00F	-0.5(4)	C00I-C00O-C00P-C00X	-176.9(3)
C007-C00F-C00P-C00O	0.2(4)	C007-C00F-C00P-C00X	176.6(3)
C00S-C00D-C00R-C00T	178.5(3)	C00H-C00D-C00R-C00T	-1.2(4)
C00A-C00M-C00S-C00D	-0.1(4)	C00R-C00D-C00S-C00M	178.6(3)
C00H-C00D-C00S-C00M	-1.7(4)	C00D-C00R-C00T-C00U	0.4(5)
C00H-C00J-C00U-C00T	-0.5(4)	C00R-C00T-C00U-C00J	0.4(5)
C00G-C00C-C00V-C00Y	0.9(5)	C00L-C00C-C00V-C00Y	179.4(3)
C00G-C00N-C00W-C00Y	0.4(5)	C00C-C00V-C00Y-C00W	0.7(5)
C00N-C00W-C00Y-C00V	-1.3(5)		

Table S8. Anisotropic atomic displacement parameters (Å^2) for L-CN.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O001	0.0333(10)	0.0504(12)	0.0277(9)	-0.0022(8)	-0.0012(7)	0.0031(9)
O002	0.0337(10)	0.0476(12)	0.0341(10)	-0.0034(9)	0.0043(8)	0.0000(9)
N003	0.0284(11)	0.0355(12)	0.0242(10)	0.0001(9)	0.0001(8)	0.0019(9)
N004	0.0304(11)	0.0331(12)	0.0304(11)	-0.0025(9)	0.0008(9)	-0.0011(10)
C005	0.0303(13)	0.0311(14)	0.0285(12)	0.0001(10)	0.0000(10)	0.0033(11)
C006	0.0344(14)	0.0336(15)	0.0261(12)	0.0003(10)	-0.0023(10)	0.0047(11)
C007	0.0292(13)	0.0304(14)	0.0302(12)	0.0003(10)	0.0026(10)	0.0049(11)
C008	0.0333(14)	0.0331(14)	0.0286(12)	0.0002(11)	0.0013(10)	0.0053(11)
C009	0.0301(13)	0.0350(15)	0.0294(13)	-0.0006(11)	-0.0006(10)	0.0068(11)
C00A	0.0348(14)	0.0347(15)	0.0341(13)	0.0006(11)	-0.0021(11)	-0.0064(12)
C00B	0.0321(14)	0.0316(14)	0.0327(13)	-0.0013(11)	-0.0002(11)	-0.0033(11)
C00C	0.0322(14)	0.0342(15)	0.0343(14)	-0.0001(11)	0.0001(11)	0.0021(11)
C00D	0.0401(15)	0.0338(15)	0.0350(14)	-0.0001(11)	-0.0011(11)	-0.0092(12)
C00E	0.0318(13)	0.0336(15)	0.0321(13)	-0.0040(11)	0.0018(11)	-0.0059(11)
C00F	0.0341(14)	0.0376(15)	0.0311(13)	0.0006(11)	0.0000(11)	0.0060(12)
C00G	0.0310(13)	0.0309(14)	0.0311(13)	-0.0003(11)	0.0002(10)	0.0002(11)
C00H	0.0387(15)	0.0312(14)	0.0316(13)	0.0024(11)	-0.0025(11)	-0.0103(12)
C00I	0.0272(13)	0.0435(16)	0.0373(14)	0.0028(12)	0.0010(11)	0.0008(12)
C00J	0.0345(14)	0.0382(16)	0.0337(14)	0.0003(12)	-0.0027(11)	-0.0058(12)
C00K	0.0358(15)	0.0457(17)	0.0268(13)	0.0019(12)	0.0029(11)	0.0048(13)
C00L	0.0306(14)	0.0432(17)	0.0356(14)	0.0018(12)	0.0041(11)	0.0013(12)
C00M	0.0375(15)	0.0396(16)	0.0373(14)	-0.0046(12)	0.0077(12)	-0.0090(13)
C00N	0.0350(15)	0.0440(17)	0.0331(14)	0.0014(12)	-0.0019(11)	-0.0035(13)
C00O	0.0305(14)	0.0472(18)	0.0374(14)	0.0026(13)	0.0040(11)	0.0007(12)
C00P	0.0367(15)	0.0444(17)	0.0323(14)	0.0034(12)	0.0082(11)	0.0048(13)
N00Q	0.0496(16)	0.095(2)	0.0376(14)	0.0018(14)	0.0024(12)	-0.0162(16)
C00R	0.0474(17)	0.0463(18)	0.0299(13)	0.0019(12)	-0.0065(12)	-0.0099(14)
C00S	0.0467(17)	0.0473(18)	0.0292(13)	-0.0027(12)	0.0009(12)	-0.0111(14)
C00T	0.0413(17)	0.0467(18)	0.0426(16)	0.0017(13)	-0.0113(13)	-0.0024(14)
C00U	0.0378(15)	0.0410(17)	0.0403(15)	0.0004(13)	-0.0061(12)	-0.0047(13)
C00V	0.0341(15)	0.0516(19)	0.0424(15)	-0.0003(14)	-0.0005(12)	-0.0057(14)
C00W	0.0439(17)	0.061(2)	0.0309(14)	0.0013(13)	-0.0041(12)	-0.0059(15)
C00X	0.0376(16)	0.058(2)	0.0368(15)	-0.0029(14)	-0.0006(12)	-0.0099(14)
C00Y	0.0358(16)	0.062(2)	0.0426(16)	-0.0003(15)	-0.0087(13)	-0.0086(15)

Table S9. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for L-CN.

	x/a	y/b	z/c	U(eq)
H002	0.5747	0.4426	0.2215	0.058
H003	0.6406	0.5958	0.3054	0.035
H006	0.7154	0.6440	0.3980	0.038
H00B	0.2953	0.5991	0.2514	0.039
H00F	0.5439	0.5407	0.4253	0.041
H00I	0.2514	0.3784	0.3077	0.043
H00J	0.1641	0.7142	0.2071	0.043
H00K	0.9706	0.8005	0.2395	0.043
H00L	1.1263	0.8993	0.2881	0.044
H00M	0.5817	0.4444	0.1012	0.046
H00N	0.8629	0.7110	0.4420	0.045
H00O	0.2026	0.3468	0.3889	0.046
H00R	0.2239	0.7044	0.0404	0.049
H00S	0.4271	0.5530	0.0516	0.049
H00T	0.0416	0.8201	0.0713	0.052
H00U	0.0120	0.8230	0.1553	0.048
H00V	1.2167	0.9509	0.3682	0.051
H00W	1.0283	0.8129	0.4883	0.054
H00Y	1.2046	0.9387	0.4519	0.056

Table S10. Hydrogen bond distances (Å) and angles (°) for L-CN.

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O002-H002···N004	0.84	1.87	2.614(3)	147.3
N003-H003···O001	0.88	1.83	2.546(3)	137.4
C00F-H00F···N00Q#2	0.95	2.47	3.419(4)	173.3
C00I-H00I···O001#1	0.95	2.51	3.279(3)	138.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, y-1/2, -z+1/2

#2 -x+1, -y+1, -z+1

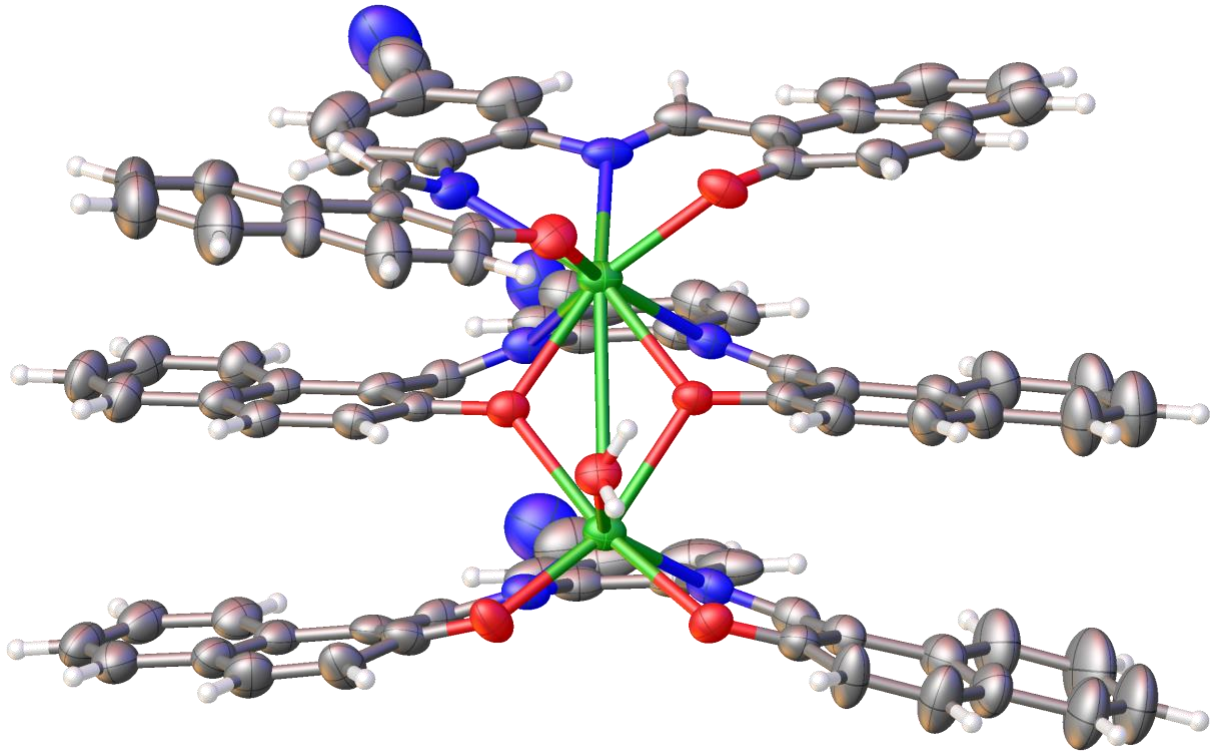


Figure S19. Projection of front view of [Er_2(L-CN)$_3$]. Carbon atoms are shown in grey, nitrogen in blue, oxygen in red, and erbium in green.

Table S11. Sample and crystal data for [Er_2(L-CN)$_3$].

Identification code	Ethan102519b	
CCDC	1964323	
Chemical formula	$C_{87}H_{55}Er_2N_9O_8$	
Formula weight	1688.92 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.010 × 0.080 × 0.136 mm	
Crystal habit	clear pale-yellow thin plate	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.3689(8) Å	α = 107.514(6)°
	b = 18.7929(18) Å	β = 95.038(5)°
	c = 18.9759(17) Å	γ = 104.652(5)°
Volume	3357.3(5) Å^3	
Z	2	

Density (calculated)	1.671 g/cm^3
Absorption coefficient	5.078 mm^{-1}
F(000)	1680

Table S12. Data collection and structure refinement for [Er$_2$(L-CN)$_3$].

Diffractometer	Bruker D8 VENTURE κ-geometry diffractometer	
Radiation source	Incoatec IμS DIAMOND microfocus sealed tube (Cu Kα, λ = 1.54178 Å)	
Theta range for data collection	2.48 to 65.32°	
Index ranges	-12<=h<=12, -22<=k<=22, -22<=l<=22	
Reflections collected	129841	
Independent reflections	11507 [R(int) = 0.0926]	
Coverage of independent reflections	99.7%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.9510 and 0.5450	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	11507 / 3 / 955	
Goodness-of-fit on F^2	1.051	
Δ/σ_{max}	0.002	
Final R indices	8493 data; I>2σ(I)	R1 = 0.0521, wR2 = 0.1357
	all data	R1 = 0.0743, wR2 = 0.1499
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0841P)^2+7.0507P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0001(0)	
Largest diff. peak and hole	2.118 and -1.499 eÅ^{-3}	
R.M.S. deviation from mean	0.122 eÅ^{-3}	

Table S13. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for $[Er_2(L\text{-}CN)_3]$.

	x/a	y/b	z/c	U(eq)
Er01	0.16134(3)	0.64772(2)	0.61886(2)	0.03266(13)
C1	0.9398(6)	0.5834(4)	0.7130(4)	0.0419(16)
Er02	0.53432(3)	0.69247(2)	0.70002(2)	0.03427(13)
C2	0.8482(7)	0.5138(4)	0.7122(4)	0.0487(18)
O1	0.6826(4)	0.6930(3)	0.6217(2)	0.0407(10)
O2	0.5086(5)	0.5649(3)	0.6630(2)	0.0430(11)
O3	0.3812(4)	0.6784(2)	0.5953(2)	0.0314(9)
C3	0.8119(7)	0.5044(5)	0.7772(4)	0.0531(18)
O4	0.3114(4)	0.6480(2)	0.7181(2)	0.0331(9)
C4	0.8632(7)	0.5652(4)	0.8470(4)	0.0457(16)
O5	0.0477(4)	0.6286(2)	0.5063(2)	0.0364(10)
C5	0.8306(8)	0.5533(5)	0.9154(4)	0.0533(18)
O6	0.9820(4)	0.5857(3)	0.6506(2)	0.0421(11)
C6	0.8813(8)	0.6126(5)	0.9826(4)	0.055(2)
O7W	0.1654(5)	0.5190(2)	0.5527(2)	0.0382(10)
C87	0.9163(10)	0.9210(6)	0.0430(6)	0.081(3)
N1	0.1819(5)	0.7761(3)	0.6082(3)	0.0376(12)
N2	0.1177(5)	0.7410(3)	0.7287(3)	0.0368(12)
N3	0.3961(10)	0.0697(6)	0.9380(6)	0.106(3)
N4	0.5461(5)	0.8235(3)	0.6865(3)	0.0350(12)
N5	0.4844(5)	0.7905(3)	0.8071(3)	0.0354(12)
N6	0.7599(8)	0.1154(4)	0.0188(4)	0.075(2)
N7	0.7563(5)	0.7781(3)	0.7730(3)	0.0384(12)
C7	0.9661(8)	0.6835(5)	0.9853(4)	0.0548(19)
N8	0.6072(5)	0.6609(3)	0.8100(3)	0.0431(14)
C8	0.9977(7)	0.6970(4)	0.9208(4)	0.0473(17)
N9	0.9789(10)	0.9786(6)	0.0955(5)	0.110(3)
C9	0.9466(6)	0.6388(4)	0.8486(4)	0.0415(15)
C10	0.9816(6)	0.6482(4)	0.7802(4)	0.0396(15)
C11	0.0541(6)	0.7232(4)	0.7804(3)	0.0417(16)
C12	0.1852(6)	0.8206(4)	0.7411(4)	0.0436(16)
C13	0.2230(7)	0.8802(4)	0.8114(4)	0.057(2)
C14	0.2943(8)	0.9559(4)	0.8146(6)	0.072(3)
C29	0.3486(11)	0.0182(6)	0.8788(6)	0.090(3)
C28	0.0580(6)	0.6631(4)	0.4560(4)	0.0384(15)

	x/a	y/b	z/c	U(eq)
C27	0.9966(8)	0.6170(4)	0.3804(4)	0.060(2)
C26	0.0007(10)	0.6485(5)	0.3254(5)	0.072(3)
C25	0.0684(8)	0.7275(5)	0.3384(5)	0.058(2)
C24	0.0741(11)	0.7587(6)	0.2793(6)	0.082(3)
C23	0.1402(13)	0.8348(7)	0.2920(7)	0.099(4)
C22	0.2045(14)	0.8817(6)	0.3637(7)	0.104(4)
C21	0.2040(11)	0.8537(5)	0.4233(6)	0.077(3)
C20	0.1311(7)	0.7751(4)	0.4120(4)	0.0511(18)
C19	0.1222(6)	0.7419(4)	0.4729(4)	0.0401(15)
C18	0.1666(6)	0.7944(4)	0.5471(4)	0.0439(16)
C17	0.2207(6)	0.8397(4)	0.6772(4)	0.0407(16)
C16	0.2930(7)	0.9156(4)	0.6853(5)	0.056(2)
C15	0.3303(8)	0.9747(5)	0.7540(6)	0.068(3)
C30	0.2899(6)	0.6364(3)	0.7827(3)	0.0306(13)
C31	0.2138(6)	0.5622(4)	0.7810(4)	0.0345(14)
C32	0.1898(6)	0.5471(4)	0.8459(4)	0.0388(14)
C33	0.2410(7)	0.6059(4)	0.9169(4)	0.0425(16)
C34	0.2161(8)	0.5900(5)	0.9840(4)	0.0507(18)
C35	0.2691(8)	0.6471(5)	0.0526(4)	0.057(2)
C36	0.3460(8)	0.7209(5)	0.0570(4)	0.0537(19)
C37	0.3700(7)	0.7382(4)	0.9929(4)	0.0452(16)
C38	0.3164(6)	0.6815(4)	0.9210(3)	0.0375(14)
C39	0.3412(6)	0.6968(4)	0.8519(3)	0.0348(14)
C40	0.4130(6)	0.7749(3)	0.8562(3)	0.0349(14)
C41	0.5537(6)	0.8711(4)	0.8184(4)	0.0404(15)
C42	0.5959(6)	0.9291(4)	0.8884(4)	0.0462(17)
C43	0.6737(7)	0.0039(4)	0.8909(4)	0.0503(19)
C57	0.4143(6)	0.7037(4)	0.5386(4)	0.0360(14)
C56	0.3699(6)	0.6510(4)	0.4642(3)	0.0383(14)
C55	0.3932(7)	0.6744(4)	0.4051(4)	0.0441(16)
C54	0.4604(7)	0.7523(4)	0.4136(4)	0.0508(18)
C53	0.4842(9)	0.7759(5)	0.3503(5)	0.072(3)
C52	0.5542(11)	0.8514(6)	0.3604(5)	0.085(3)
C51	0.6027(10)	0.9053(5)	0.4314(5)	0.078(3)
C50	0.5836(8)	0.8846(5)	0.4938(5)	0.062(2)
C49	0.5090(7)	0.8070(4)	0.4870(4)	0.0457(16)
C48	0.4852(6)	0.7812(4)	0.5501(4)	0.0364(14)

	x/a	y/b	z/c	U(eq)
C47	0.5278(6)	0.8381(4)	0.6254(4)	0.0426(16)
C46	0.5884(6)	0.8871(4)	0.7540(4)	0.0378(14)
C45	0.6683(7)	0.9612(4)	0.7611(4)	0.0494(18)
C44	0.7102(7)	0.0203(4)	0.8286(4)	0.0505(18)
C58	0.7189(8)	0.0653(5)	0.9615(5)	0.058(2)
C59	0.7657(6)	0.7516(4)	0.6125(4)	0.0384(15)
C60	0.7872(6)	0.7473(4)	0.5378(4)	0.0451(17)
C61	0.8639(7)	0.8090(4)	0.5223(4)	0.0479(17)
C62	0.9317(6)	0.8813(4)	0.5809(4)	0.0461(17)
C63	0.0060(7)	0.9459(4)	0.5646(5)	0.057(2)
C64	0.0665(8)	0.0159(4)	0.6208(5)	0.059(2)
C65	0.0553(8)	0.0228(5)	0.6940(5)	0.061(2)
C66	0.9854(7)	0.9595(4)	0.7133(4)	0.0495(18)
C67	0.9219(6)	0.8867(4)	0.6560(4)	0.0451(16)
C68	0.8424(6)	0.8198(4)	0.6719(4)	0.0402(15)
C69	0.8450(6)	0.8227(4)	0.7485(4)	0.0432(16)
C70	0.7722(7)	0.7866(4)	0.8513(4)	0.0472(18)
C71	0.8545(8)	0.8534(5)	0.9078(4)	0.060(2)
C72	0.8465(9)	0.8569(6)	0.9835(4)	0.070(3)
C73	0.7600(10)	0.7986(6)	0.0013(5)	0.072(3)
C74	0.6825(9)	0.7341(5)	0.9445(4)	0.059(2)
C75	0.6885(7)	0.7261(5)	0.8698(4)	0.0507(19)
C76	0.5747(7)	0.5939(4)	0.8206(4)	0.0454(17)
C77	0.4904(7)	0.5211(4)	0.7682(4)	0.0415(15)
C78	0.4389(7)	0.4558(5)	0.7952(4)	0.0491(18)
C79	0.4555(8)	0.4634(6)	0.8719(4)	0.061(2)
C80	0.4034(9)	0.3996(7)	0.8939(5)	0.074(3)
C81	0.3317(11)	0.3281(6)	0.8427(6)	0.081(3)
C82	0.3113(11)	0.3213(6)	0.7693(6)	0.080(3)
C83	0.3646(9)	0.3836(5)	0.7439(4)	0.057(2)
C84	0.3423(10)	0.3754(5)	0.6666(5)	0.066(2)
C85	0.3897(8)	0.4354(4)	0.6412(4)	0.0527(19)
C86	0.4652(7)	0.5109(4)	0.6909(4)	0.0410(15)

Table S14. Bond lengths (Å) for [Er_2(L-CN)$_3$].

Er01-O6	2.167(4)	Er01-O5	2.228(4)

Er01-O3	2.324(4)	Er01-O4	2.333(4)
Er01-O7W	2.379(4)	Er01-N1	2.439(5)
Er01-N2	2.447(5)	Er01-Er02	3.8164(6)
C1-O6	1.307(8)	C1-C2	1.404(10)
C1-C10	1.415(9)	Er02-O2	2.223(4)
Er02-O1	2.231(4)	Er02-O3	2.337(4)
Er02-O4	2.344(4)	Er02-N8	2.444(6)
Er02-N7	2.456(5)	Er02-N5	2.491(5)
Er02-N4	2.525(5)	C2-C3	1.368(10)
C2-H2	0.95	O1-C59	1.283(8)
O2-C86	1.284(8)	O3-C57	1.338(7)
C3-C4	1.415(10)	C3-H3	0.95
O4-C30	1.336(7)	C4-C9	1.424(10)
C4-C5	1.437(10)	O5-C28	1.302(8)
C5-C6	1.369(10)	C5-H5	0.95
C6-C7	1.382(11)	C6-H6	0.95
O7W-H7WA	0.85(2)	O7W-H7WB	0.84(2)
C87-N9	1.211(12)	C87-C72	1.360(12)
N1-C18	1.313(9)	N1-C17	1.423(8)
N2-C11	1.308(8)	N2-C12	1.419(8)
N3-C29	1.205(12)	N4-C47	1.280(8)
N4-C46	1.406(8)	N5-C40	1.296(8)
N5-C41	1.443(8)	N6-C58	1.162(10)
N7-C69	1.298(9)	N7-C70	1.436(9)
C7-C8	1.373(10)	C7-H7	0.95
N8-C76	1.300(9)	N8-C75	1.405(9)
C8-C9	1.425(9)	C8-H8	0.95
C9-C10	1.425(9)	C10-C11	1.420(10)
C11-H11	0.95	C12-C13	1.405(9)
C12-C17	1.417(10)	C13-C14	1.408(12)
C13-H13	0.95	C14-C15	1.358(14)
C14-C29	1.362(12)	C28-C19	1.385(9)
C28-C27	1.424(10)	C27-C26	1.344(10)
C27-H27	0.95	C26-C25	1.406(11)
C26-H26	0.95	C25-C20	1.403(11)
C25-C24	1.412(11)	C24-C23	1.357(13)
C24-H24	0.95	C23-C22	1.376(15)
C23-H23	0.95	C22-C21	1.382(13)

C22-H22	0.95	C21-C20	1.419(11)
C21-H21	0.95	C20-C19	1.468(10)
C19-C18	1.410(9)	C18-H18	0.95
C17-C16	1.389(9)	C16-C15	1.380(12)
C16-H16	0.95	C15-H15	0.95
C30-C39	1.402(8)	C30-C31	1.408(8)
C31-C32	1.374(9)	C31-H31	0.95
C32-C33	1.414(9)	C32-H32	0.95
C33-C38	1.413(10)	C33-C34	1.422(9)
C34-C35	1.372(10)	C34-H34	0.95
C35-C36	1.388(11)	C35-H35	0.95
C36-C37	1.379(10)	C36-H36	0.95
C37-C38	1.413(9)	C37-H37	0.95
C38-C39	1.456(9)	C39-C40	1.441(9)
C40-H40	0.95	C41-C42	1.389(9)
C41-C46	1.398(9)	C42-C43	1.417(10)
C42-H42	0.95	C43-C44	1.369(11)
C43-C58	1.425(10)	C57-C48	1.396(9)
C57-C56	1.414(9)	C56-C55	1.342(9)
C56-H56	0.95	C55-C54	1.405(10)
C55-H55	0.95	C54-C49	1.415(10)
C54-C53	1.420(10)	C53-C52	1.367(12)
C53-H53	0.95	C52-C51	1.378(13)
C52-H52	0.95	C51-C50	1.368(11)
C51-H51	0.95	C50-C49	1.429(10)
C50-H50	0.95	C49-C48	1.440(9)
C48-C47	1.453(9)	C47-H47	0.95
C46-C45	1.389(9)	C45-C44	1.366(10)
C45-H45	0.95	C44-H44	0.95
C59-C68	1.416(9)	C59-C60	1.436(9)
C60-C61	1.357(10)	C60-H60	0.95
C61-C62	1.431(10)	C61-H61	0.95
C62-C63	1.400(10)	C62-C67	1.412(10)
C63-C64	1.372(11)	C63-H63	0.95
C64-C65	1.374(11)	C64-H64	0.95
C65-C66	1.395(11)	C65-H65	0.95
C66-C67	1.418(9)	C66-H66	0.95
C67-C68	1.449(10)	C68-C69	1.436(10)

C69-H69	0.95	C70-C71	1.393(10)
C70-C75	1.401(11)	C71-C72	1.427(12)
C71-H71	0.95	C72-C73	1.378(13)
C73-C74	1.358(12)	C73-H73	0.95
C74-C75	1.389(10)	C74-H74	0.95
C76-C77	1.431(10)	C76-H76	0.95
C77-C86	1.412(9)	C77-C78	1.467(10)
C78-C83	1.388(11)	C78-C79	1.410(10)
C79-C80	1.384(12)	C79-H79	0.95
C80-C81	1.372(13)	C80-H80	0.95
C81-C82	1.351(12)	C81-H81	0.95
C82-C83	1.404(11)	C82-H82	0.95
C83-C84	1.420(11)	C84-C85	1.354(11)
C84-H84	0.95	C85-C86	1.421(10)

Table S15. Bond angles (°) for [Er_2(L-CN)$_3$].

O6-Er01-O5	91.93(16)	O6-Er01-O3	158.68(16)
O5-Er01-O3	99.48(15)	O6-Er01-O4	94.78(15)
O5-Er01-O4	165.07(15)	O3-Er01-O4	70.22(14)
O6-Er01-O7W	82.77(17)	O5-Er01-O7W	79.44(15)
O3-Er01-O7W	81.71(15)	O4-Er01-O7W	88.18(14)
O6-Er01-N1	120.50(17)	O5-Er01-N1	72.85(16)
O3-Er01-N1	80.29(15)	O4-Er01-N1	114.51(16)
O7W-Er01-N1	143.73(17)	O6-Er01-N2	73.33(17)
O5-Er01-N2	118.29(16)	O3-Er01-N2	115.62(15)
O4-Er01-N2	76.48(15)	O7W-Er01-N2	150.14(17)
N1-Er01-N2	65.88(18)	O6-Er01-Er02	129.62(12)
O5-Er01-Er02	134.45(11)	O3-Er01-Er02	35.14(10)
O4-Er01-Er02	35.41(10)	O7W-Er01-Er02	87.40(11)
N1-Er01-Er02	95.48(12)	N2-Er01-Er02	94.12(12)
O6-C1-C2	118.2(6)	O6-C1-C10	122.6(6)
C2-C1-C10	119.3(6)	O2-Er02-O1	83.83(16)
O2-Er02-O3	91.76(15)	O1-Er02-O3	83.73(15)
O2-Er02-O4	80.54(15)	O1-Er02-O4	148.63(14)
O3-Er02-O4	69.81(14)	O2-Er02-N8	72.37(18)
O1-Er02-N8	113.51(17)	O3-Er02-N8	154.29(18)
O4-Er02-N8	87.34(16)	O2-Er02-N7	116.40(17)

O1-Er02-N7	72.01(16)	O3-Er02-N7	139.53(17)
O4-Er02-N7	139.36(15)	N8-Er02-N7	66.1(2)
O2-Er02-N5	136.66(17)	O1-Er02-N5	136.57(16)
O3-Er02-N5	105.36(15)	O4-Er02-N5	69.23(15)
N8-Er02-N5	75.82(17)	N7-Er02-N5	74.58(16)
O2-Er02-N4	157.24(17)	O1-Er02-N4	81.92(16)
O3-Er02-N4	69.14(15)	O4-Er02-N4	103.06(15)
N8-Er02-N4	129.84(18)	N7-Er02-N4	75.63(17)
N5-Er02-N4	63.35(17)	O2-Er02-Er01	88.88(12)
O1-Er02-Er01	117.98(11)	O3-Er02-Er01	34.92(10)
O4-Er02-Er01	35.22(10)	N8-Er02-Er01	122.36(14)
N7-Er02-Er01	154.32(12)	N5-Er02-Er01	83.94(11)
N4-Er02-Er01	82.30(11)	C3-C2-C1	121.0(7)
C3-C2-H2	119.5	C1-C2-H2	119.5
C59-O1-Er02	128.8(4)	C86-O2-Er02	134.3(4)
C57-O3-Er01	123.0(3)	C57-O3-Er02	124.9(3)
Er01-O3-Er02	109.94(16)	C2-C3-C4	121.0(7)
C2-C3-H3	119.5	C4-C3-H3	119.5
C30-O4-Er01	130.8(3)	C30-O4-Er02	119.2(3)
Er01-O4-Er02	109.38(16)	C3-C4-C9	119.1(6)
C3-C4-C5	120.5(7)	C9-C4-C5	120.3(6)
C28-O5-Er01	136.9(4)	C6-C5-C4	119.9(8)
C6-C5-H5	120.1	C4-C5-H5	120.1
C1-O6-Er01	136.9(4)	C5-C6-C7	120.5(7)
C5-C6-H6	119.8	C7-C6-H6	119.8
Er01-O7W-H7WA	130.(8)	Er01-O7W-H7WB	120.(10)
H7WA-O7W-H7WB	88.(3)	N9-C87-C72	179.3(13)
C18-N1-C17	115.9(6)	C18-N1-Er01	128.5(4)
C17-N1-Er01	115.6(4)	C11-N2-C12	118.5(5)
C11-N2-Er01	125.7(4)	C12-N2-Er01	115.2(4)
C47-N4-C46	117.7(6)	C47-N4-Er02	127.2(4)
C46-N4-Er02	114.9(4)	C40-N5-C41	118.5(5)
C40-N5-Er02	125.6(4)	C41-N5-Er02	115.6(4)
C69-N7-C70	120.4(6)	C69-N7-Er02	124.8(4)
C70-N7-Er02	113.9(4)	C8-C7-C6	121.0(7)
C8-C7-H7	119.5	C6-C7-H7	119.5
C76-N8-C75	117.8(6)	C76-N8-Er02	128.5(5)
C75-N8-Er02	113.6(5)	C7-C8-C9	121.9(7)

C7-C8-H8	119.0	C9-C8-H8	119.0
C4-C9-C8	116.4(6)	C4-C9-C10	119.1(6)
C8-C9-C10	124.3(7)	C1-C10-C11	121.0(6)
C1-C10-C9	119.7(6)	C11-C10-C9	119.2(6)
N2-C11-C10	128.1(6)	N2-C11-H11	116.0
C10-C11-H11	116.0	C13-C12-C17	118.5(7)
C13-C12-N2	125.2(7)	C17-C12-N2	116.3(6)
C12-C13-C14	118.2(9)	C12-C13-H13	120.9
C14-C13-H13	120.9	C15-C14-C29	110.4(10)
C15-C14-C13	123.9(8)	C29-C14-C13	125.3(11)
N3-C29-C14	175.6(14)	O5-C28-C19	123.4(6)
O5-C28-C27	117.6(6)	C19-C28-C27	119.0(6)
C26-C27-C28	121.2(7)	C26-C27-H27	119.4
C28-C27-H27	119.4	C27-C26-C25	122.5(8)
C27-C26-H26	118.7	C25-C26-H26	118.7
C20-C25-C26	118.3(7)	C20-C25-C24	120.3(8)
C26-C25-C24	121.4(8)	C23-C24-C25	121.2(9)
C23-C24-H24	119.4	C25-C24-H24	119.4
C24-C23-C22	119.0(9)	C24-C23-H23	120.5
C22-C23-H23	120.5	C23-C22-C21	122.1(10)
C23-C22-H22	119.0	C21-C22-H22	119.0
C22-C21-C20	120.0(9)	C22-C21-H21	120.0
C20-C21-H21	120.0	C25-C20-C21	117.3(7)
C25-C20-C19	119.5(6)	C21-C20-C19	123.1(7)
C28-C19-C18	123.0(6)	C28-C19-C20	119.3(6)
C18-C19-C20	117.3(6)	N1-C18-C19	126.5(6)
N1-C18-H18	116.8	C19-C18-H18	116.8
C16-C17-C12	119.8(7)	C16-C17-N1	124.8(7)
C12-C17-N1	115.4(6)	C15-C16-C17	122.3(9)
C15-C16-H16	118.9	C17-C16-H16	118.9
C14-C15-C16	117.3(8)	C14-C15-H15	121.3
C16-C15-H15	121.3	O4-C30-C39	121.3(6)
O4-C30-C31	119.1(5)	C39-C30-C31	119.7(6)
C32-C31-C30	121.3(6)	C32-C31-H31	119.3
C30-C31-H31	119.3	C31-C32-C33	121.0(6)
C31-C32-H32	119.5	C33-C32-H32	119.5
C38-C33-C32	119.4(6)	C38-C33-C34	119.8(6)
C32-C33-C34	120.8(7)	C35-C34-C33	120.2(7)

C35-C34-H34	119.9	C33-C34-H34	119.9
C34-C35-C36	120.3(7)	C34-C35-H35	119.9
C36-C35-H35	119.9	C37-C36-C35	120.8(7)
C37-C36-H36	119.6	C35-C36-H36	119.6
C36-C37-C38	120.9(7)	C36-C37-H37	119.6
C38-C37-H37	119.6	C33-C38-C37	118.1(6)
C33-C38-C39	119.1(6)	C37-C38-C39	122.7(6)
C30-C39-C40	121.6(6)	C30-C39-C38	119.5(6)
C40-C39-C38	118.9(5)	N5-C40-C39	123.7(6)
N5-C40-H40	118.1	C39-C40-H40	118.1
C42-C41-C46	120.5(6)	C42-C41-N5	123.8(7)
C46-C41-N5	115.4(5)	C41-C42-C43	117.1(7)
C41-C42-H42	121.5	C43-C42-H42	121.5
C44-C43-C42	123.2(7)	C44-C43-C58	117.7(7)
C42-C43-C58	119.0(8)	O3-C57-C48	122.3(6)
O3-C57-C56	118.9(6)	C48-C57-C56	118.8(6)
C55-C56-C57	121.3(6)	C55-C56-H56	119.3
C57-C56-H56	119.3	C56-C55-C54	122.1(6)
C56-C55-H55	119.0	C54-C55-H55	119.0
C55-C54-C49	118.8(6)	C55-C54-C53	121.2(7)
C49-C54-C53	119.9(7)	C52-C53-C54	120.0(8)
C52-C53-H53	120.0	C54-C53-H53	120.0
C53-C52-C51	120.8(9)	C53-C52-H52	119.6
C51-C52-H52	119.6	C50-C51-C52	121.0(8)
C50-C51-H51	119.5	C52-C51-H51	119.5
C51-C50-C49	120.8(8)	C51-C50-H50	119.6
C49-C50-H50	119.6	C54-C49-C50	117.4(7)
C54-C49-C48	118.7(6)	C50-C49-C48	123.8(7)
C57-C48-C49	120.2(6)	C57-C48-C47	120.8(6)
C49-C48-C47	118.9(6)	N4-C47-C48	126.3(6)
N4-C47-H47	116.9	C48-C47-H47	116.9
C45-C46-C41	119.2(6)	C45-C46-N4	124.7(6)
C41-C46-N4	116.0(6)	C44-C45-C46	122.3(7)
C44-C45-H45	118.8	C46-C45-H45	118.8
C45-C44-C43	117.7(7)	C45-C44-H44	121.2
C43-C44-H44	121.2	N6-C58-C43	177.9(9)
O1-C59-C68	124.2(6)	O1-C59-C60	118.6(6)
C68-C59-C60	117.2(6)	C61-C60-C59	122.3(6)

C61-C60-H60	118.8	C59-C60-H60	118.8
C60-C61-C62	121.0(7)	C60-C61-H61	119.5
C62-C61-H61	119.5	C63-C62-C67	120.2(7)
C63-C62-C61	121.0(7)	C67-C62-C61	118.8(7)
C64-C63-C62	120.6(8)	C64-C63-H63	119.7
C62-C63-H63	119.7	C63-C64-C65	119.9(8)
C63-C64-H64	120.0	C65-C64-H64	120.0
C64-C65-C66	121.5(7)	C64-C65-H65	119.3
C66-C65-H65	119.3	C65-C66-C67	119.4(7)
C65-C66-H66	120.3	C67-C66-H66	120.3
C62-C67-C66	118.2(7)	C62-C67-C68	119.6(6)
C66-C67-C68	122.1(7)	C59-C68-C69	120.3(6)
C59-C68-C67	120.4(6)	C69-C68-C67	119.3(6)
N7-C69-C68	126.2(6)	N7-C69-H69	116.9
C68-C69-H69	116.9	C71-C70-C75	120.1(7)
C71-C70-N7	123.7(8)	C75-C70-N7	115.9(6)
C70-C71-C72	116.9(9)	C70-C71-H71	121.5
C72-C71-H71	121.5	C87-C72-C73	115.2(9)
C87-C72-C71	122.0(11)	C73-C72-C71	122.7(7)
C74-C73-C72	118.5(8)	C74-C73-H73	120.7
C72-C73-H73	120.7	C73-C74-C75	121.6(9)
C73-C74-H74	119.2	C75-C74-H74	119.2
C74-C75-C70	120.1(7)	C74-C75-N8	122.7(8)
C70-C75-N8	117.1(6)	N8-C76-C77	126.7(6)
N8-C76-H76	116.6	C77-C76-H76	116.6
C86-C77-C76	120.4(6)	C86-C77-C78	120.5(6)
C76-C77-C78	118.9(6)	C83-C78-C79	117.6(7)
C83-C78-C77	119.2(6)	C79-C78-C77	123.1(7)
C80-C79-C78	120.3(9)	C80-C79-H79	119.8
C78-C79-H79	119.8	C81-C80-C79	121.6(8)
C81-C80-H80	119.2	C79-C80-H80	119.2
C82-C81-C80	118.2(9)	C82-C81-H81	120.9
C80-C81-H81	120.9	C81-C82-C83	122.4(10)
C81-C82-H82	118.8	C83-C82-H82	118.8
C78-C83-C82	119.7(8)	C78-C83-C84	118.6(7)
C82-C83-C84	121.7(8)	C85-C84-C83	122.5(8)
C85-C84-H84	118.7	C83-C84-H84	118.7
C84-C85-C86	121.6(7)	C84-C85-H85	119.2

C86-C85-H85	119.2	O2-C86-C77	124.1(6)
O2-C86-C85	118.4(6)	C77-C86-C85	117.5(6)

Table S16. Torsion angles (°) for $[Er_2(L\text{-}CN)_3]$.

O6-C1-C2-C3	172.6(7)	C10-C1-C2-C3	-8.2(10)
C1-C2-C3-C4	1.4(11)	C2-C3-C4-C9	4.3(11)
C2-C3-C4-C5	-176.4(7)	C3-C4-C5-C6	179.9(7)
C9-C4-C5-C6	-0.8(10)	C2-C1-O6-Er01	-151.9(5)
C10-C1-O6-Er01	28.9(10)	C4-C5-C6-C7	-1.4(11)
C5-C6-C7-C8	2.3(11)	C6-C7-C8-C9	-0.9(11)
C3-C4-C9-C8	-178.6(6)	C5-C4-C9-C8	2.1(9)
C3-C4-C9-C10	-3.1(9)	C5-C4-C9-C10	177.6(6)
C7-C8-C9-C4	-1.3(10)	C7-C8-C9-C10	-176.5(6)
O6-C1-C10-C11	10.6(9)	C2-C1-C10-C11	-168.6(6)
O6-C1-C10-C9	-171.6(6)	C2-C1-C10-C9	9.2(9)
C4-C9-C10-C1	-3.6(9)	C8-C9-C10-C1	171.5(6)
C4-C9-C10-C11	174.2(6)	C8-C9-C10-C11	-10.6(9)
C12-N2-C11-C10	-179.4(6)	Er01-N2-C11-C10	-9.1(9)
C1-C10-C11-N2	-16.9(10)	C9-C10-C11-N2	165.3(6)
C11-N2-C12-C13	19.0(9)	Er01-N2-C12-C13	-152.3(5)
C11-N2-C12-C17	-163.6(6)	Er01-N2-C12-C17	25.2(7)
C17-C12-C13-C14	0.1(9)	N2-C12-C13-C14	177.5(6)
C12-C13-C14-C15	-0.9(11)	C12-C13-C14-C29	-173.7(8)
Er01-O5-C28-C19	-25.5(10)	Er01-O5-C28-C27	156.2(5)
O5-C28-C27-C26	178.9(8)	C19-C28-C27-C26	0.5(12)
C28-C27-C26-C25	1.8(15)	C27-C26-C25-C20	-1.5(14)
C27-C26-C25-C24	178.4(10)	C20-C25-C24-C23	0.3(16)
C26-C25-C24-C23	-179.6(11)	C25-C24-C23-C22	1.2(18)
C24-C23-C22-C21	0.(2)	C23-C22-C21-C20	-2.5(19)
C26-C25-C20-C21	177.2(9)	C24-C25-C20-C21	-2.7(13)
C26-C25-C20-C19	-1.1(12)	C24-C25-C20-C19	179.0(8)
C22-C21-C20-C25	3.8(14)	C22-C21-C20-C19	-178.0(9)
O5-C28-C19-C18	-8.7(10)	C27-C28-C19-C18	169.6(7)
O5-C28-C19-C20	178.7(6)	C27-C28-C19-C20	-3.0(10)
C25-C20-C19-C28	3.3(10)	C21-C20-C19-C28	-174.9(8)
C25-C20-C19-C18	-169.7(7)	C21-C20-C19-C18	12.2(11)
C17-N1-C18-C19	-176.5(6)	Er01-N1-C18-C19	6.2(10)

C28-C19-C18-N1	15.9(11)	C20-C19-C18-N1	-171.4(6)
C13-C12-C17-C16	0.9(9)	N2-C12-C17-C16	-176.7(6)
C13-C12-C17-N1	178.6(5)	N2-C12-C17-N1	0.9(8)
C18-N1-C17-C16	-27.0(9)	Er01-N1-C17-C16	150.7(5)
C18-N1-C17-C12	155.5(6)	Er01-N1-C17-C12	-26.8(6)
C12-C17-C16-C15	-1.2(10)	N1-C17-C16-C15	-178.7(6)
C29-C14-C15-C16	174.4(7)	C13-C14-C15-C16	0.6(12)
C17-C16-C15-C14	0.5(11)	Er01-O4-C30-C39	-113.2(5)
Er02-O4-C30-C39	57.4(6)	Er01-O4-C30-C31	66.5(7)
Er02-O4-C30-C31	-122.9(5)	O4-C30-C31-C32	179.5(5)
C39-C30-C31-C32	-0.8(9)	C30-C31-C32-C33	0.0(9)
C31-C32-C33-C38	0.8(9)	C31-C32-C33-C34	-179.9(6)
C38-C33-C34-C35	-2.3(10)	C32-C33-C34-C35	178.5(7)
C33-C34-C35-C36	0.7(12)	C34-C35-C36-C37	0.3(12)
C35-C36-C37-C38	0.3(11)	C32-C33-C38-C37	-178.0(6)
C34-C33-C38-C37	2.7(9)	C32-C33-C38-C39	-0.8(9)
C34-C33-C38-C39	179.9(6)	C36-C37-C38-C33	-1.8(10)
C36-C37-C38-C39	-178.9(6)	O4-C30-C39-C40	3.3(8)
C31-C30-C39-C40	-176.4(5)	O4-C30-C39-C38	-179.4(5)
C31-C30-C39-C38	0.9(8)	C33-C38-C39-C30	-0.1(8)
C37-C38-C39-C30	177.0(6)	C33-C38-C39-C40	177.3(6)
C37-C38-C39-C40	-5.7(9)	C41-N5-C40-C39	-178.9(5)
Er02-N5-C40-C39	-5.8(8)	C30-C39-C40-N5	-30.0(9)
C38-C39-C40-N5	152.7(6)	C40-N5-C41-C42	27.1(9)
Er02-N5-C41-C42	-146.7(5)	C40-N5-C41-C46	-158.7(6)
Er02-N5-C41-C46	27.5(6)	C46-C41-C42-C43	0.4(9)
N5-C41-C42-C43	174.3(6)	C41-C42-C43-C44	-1.3(10)
C41-C42-C43-C58	179.8(6)	Er01-O3-C57-C48	107.0(6)
Er02-O3-C57-C48	-54.8(7)	Er01-O3-C57-C56	-69.7(6)
Er02-O3-C57-C56	128.5(5)	O3-C57-C56-C55	176.0(6)
C48-C57-C56-C55	-0.7(9)	C57-C56-C55-C54	-1.2(10)
C56-C55-C54-C49	2.2(11)	C56-C55-C54-C53	-180.0(8)
C55-C54-C53-C52	-177.6(9)	C49-C54-C53-C52	0.2(14)
C54-C53-C52-C51	0.1(17)	C53-C52-C51-C50	0.8(17)
C52-C51-C50-C49	-2.1(15)	C55-C54-C49-C50	176.5(7)
C53-C54-C49-C50	-1.3(11)	C55-C54-C49-C48	-1.3(10)
C53-C54-C49-C48	-179.1(7)	C51-C50-C49-C54	2.3(12)
C51-C50-C49-C48	179.9(8)	O3-C57-C48-C49	-175.0(5)

C56-C57-C48-C49	1.7(9)	O3-C57-C48-C47	0.7(9)
C56-C57-C48-C47	177.4(6)	C54-C49-C48-C57	-0.6(9)
C50-C49-C48-C57	-178.2(7)	C54-C49-C48-C47	-176.4(6)
C50-C49-C48-C47	6.0(10)	C46-N4-C47-C48	179.7(6)
Er02-N4-C47-C48	5.4(9)	C57-C48-C47-N4	23.2(10)
C49-C48-C47-N4	-161.1(6)	C42-C41-C46-C45	1.4(9)
N5-C41-C46-C45	-172.9(6)	C42-C41-C46-N4	177.1(6)
N5-C41-C46-N4	2.7(8)	C47-N4-C46-C45	-30.7(9)
Er02-N4-C46-C45	144.2(6)	C47-N4-C46-C41	153.9(6)
Er02-N4-C46-C41	-31.2(6)	C41-C46-C45-C44	-2.6(10)
N4-C46-C45-C44	-177.8(6)	C46-C45-C44-C43	1.7(11)
C42-C43-C44-C45	0.3(11)	C58-C43-C44-C45	179.1(7)
Er02-O1-C59-C68	41.2(9)	Er02-O1-C59-C60	-141.3(5)
O1-C59-C60-C61	174.0(6)	C68-C59-C60-C61	-8.3(10)
C59-C60-C61-C62	2.3(10)	C60-C61-C62-C63	-177.3(7)
C60-C61-C62-C67	2.4(10)	C67-C62-C63-C64	-2.1(11)
C61-C62-C63-C64	177.5(7)	C62-C63-C64-C65	0.6(12)
C63-C64-C65-C66	1.2(12)	C64-C65-C66-C67	-1.4(11)
C63-C62-C67-C66	1.9(10)	C61-C62-C67-C66	-177.7(6)
C63-C62-C67-C68	178.8(6)	C61-C62-C67-C68	-0.8(9)
C65-C66-C67-C62	-0.2(10)	C65-C66-C67-C68	-177.0(6)
O1-C59-C68-C69	8.8(9)	C60-C59-C68-C69	-168.8(6)
O1-C59-C68-C67	-172.8(6)	C60-C59-C68-C67	9.7(9)
C62-C67-C68-C59	-5.3(9)	C66-C67-C68-C59	171.4(6)
C62-C67-C68-C69	173.1(6)	C66-C67-C68-C69	-10.1(9)
C70-N7-C69-C68	179.1(6)	Er02-N7-C69-C68	-12.7(9)
C59-C68-C69-N7	-20.5(10)	C67-C68-C69-N7	161.1(6)
C69-N7-C70-C71	19.1(9)	Er02-N7-C70-C71	-150.3(5)
C69-N7-C70-C75	-167.1(6)	Er02-N7-C70-C75	23.4(7)
C75-C70-C71-C72	-1.2(10)	N7-C70-C71-C72	172.2(6)
C70-C71-C72-C87	-176.2(8)	C70-C71-C72-C73	-1.4(11)
C87-C72-C73-C74	177.2(8)	C71-C72-C73-C74	2.1(13)
C72-C73-C74-C75	-0.2(12)	C73-C74-C75-C70	-2.3(11)
C73-C74-C75-N8	-178.5(7)	C71-C70-C75-C74	3.0(10)
N7-C70-C75-C74	-170.9(6)	C71-C70-C75-N8	179.4(6)
N7-C70-C75-N8	5.5(8)	C76-N8-C75-C74	-32.2(9)
Er02-N8-C75-C74	144.4(6)	C76-N8-C75-C70	151.6(6)
Er02-N8-C75-C70	-31.8(7)	C75-N8-C76-C77	178.1(6)

Er02-N8-C76-C77	2.1(10)	N8-C76-C77-C86	18.7(10)
N8-C76-C77-C78	-165.8(6)	C86-C77-C78-C83	-0.1(10)
C76-C77-C78-C83	-175.7(6)	C86-C77-C78-C79	-177.0(6)
C76-C77-C78-C79	7.4(10)	C83-C78-C79-C80	2.5(11)
C77-C78-C79-C80	179.4(7)	C78-C79-C80-C81	-1.7(13)
C79-C80-C81-C82	-0.6(15)	C80-C81-C82-C83	2.2(16)
C79-C78-C83-C82	-1.0(11)	C77-C78-C83-C82	-178.1(7)
C79-C78-C83-C84	177.6(7)	C77-C78-C83-C84	0.6(11)
C81-C82-C83-C78	-1.4(15)	C81-C82-C83-C84	-180.0(10)
C78-C83-C84-C85	-0.5(13)	C82-C83-C84-C85	178.1(9)
C83-C84-C85-C86	-0.1(13)	Er02-O2-C86-C77	-37.8(10)
Er02-O2-C86-C85	143.7(5)	C76-C77-C86-O2	-3.5(10)
C78-C77-C86-O2	-179.0(6)	C76-C77-C86-C85	175.1(6)
C78-C77-C86-C85	-0.4(9)	C84-C85-C86-O2	179.1(7)
C84-C85-C86-C77	0.5(11)		

Table S17. Anisotropic atomic displacement parameters (Å^2) for [Er$_2$(L-CN)$_3$].
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er01	0.0279(2)	0.0292(2)	0.0337(2)	0.00325(15)	0.00091(15)	0.00635(15)
C1	0.025(3)	0.052(4)	0.041(4)	0.007(3)	0.001(3)	0.010(3)
Er02	0.0300(2)	0.0342(2)	0.0326(2)	0.00190(16)	0.00103(15)	0.01188(16)
C2	0.035(4)	0.057(4)	0.038(4)	0.007(3)	-0.001(3)	-0.002(3)
O1	0.028(2)	0.039(2)	0.044(3)	0.001(2)	0.0059(19)	0.0053(19)
O2	0.052(3)	0.036(2)	0.040(3)	0.004(2)	0.010(2)	0.021(2)
O3	0.024(2)	0.032(2)	0.032(2)	0.0059(18)	0.0004(16)	0.0059(17)
C3	0.041(4)	0.058(5)	0.051(4)	0.016(4)	-0.003(3)	0.005(3)
O4	0.030(2)	0.033(2)	0.030(2)	0.0037(17)	-0.0005(17)	0.0085(18)
C4	0.041(4)	0.060(5)	0.036(4)	0.013(3)	0.004(3)	0.019(3)
O5	0.034(2)	0.031(2)	0.037(2)	0.0072(18)	-0.0029(18)	0.0045(18)
C5	0.050(4)	0.067(5)	0.053(4)	0.025(4)	0.011(3)	0.027(4)
O6	0.031(2)	0.050(3)	0.031(2)	0.004(2)	0.0047(18)	0.000(2)
C6	0.061(5)	0.078(6)	0.038(4)	0.022(4)	0.008(3)	0.035(4)
O7W	0.041(3)	0.027(2)	0.041(3)	0.0041(19)	0.004(2)	0.011(2)
C87	0.073(6)	0.084(7)	0.078(7)	0.021(6)	0.011(5)	0.016(5)
N1	0.027(3)	0.030(3)	0.049(3)	0.007(2)	0.006(2)	0.005(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	0.031(3)	0.036(3)	0.038(3)	0.001(2)	0.003(2)	0.014(2)
N3	0.106(7)	0.088(7)	0.101(7)	0.007(6)	0.012(6)	0.020(6)
N4	0.028(3)	0.036(3)	0.036(3)	0.004(2)	0.004(2)	0.010(2)
N5	0.031(3)	0.030(3)	0.034(3)	-0.002(2)	-0.003(2)	0.009(2)
N6	0.089(6)	0.054(4)	0.057(4)	-0.004(4)	0.006(4)	0.010(4)
N7	0.027(3)	0.042(3)	0.035(3)	-0.003(2)	-0.003(2)	0.015(2)
C7	0.059(5)	0.072(5)	0.039(4)	0.013(4)	0.006(3)	0.037(4)
N8	0.041(3)	0.057(4)	0.031(3)	0.006(3)	0.002(2)	0.026(3)
C8	0.050(4)	0.049(4)	0.043(4)	0.007(3)	0.008(3)	0.026(3)
N9	0.092(7)	0.107(7)	0.082(6)	-0.001(6)	0.002(5)	-0.009(6)
C9	0.035(3)	0.053(4)	0.039(4)	0.011(3)	0.006(3)	0.023(3)
C10	0.026(3)	0.047(4)	0.044(4)	0.008(3)	0.003(3)	0.018(3)
C11	0.040(4)	0.049(4)	0.028(3)	-0.003(3)	-0.002(3)	0.021(3)
C12	0.034(3)	0.038(4)	0.050(4)	0.000(3)	-0.001(3)	0.018(3)
C13	0.044(4)	0.055(5)	0.058(5)	-0.007(4)	-0.013(3)	0.028(4)
C14	0.048(5)	0.027(4)	0.103(7)	-0.023(4)	-0.035(5)	0.018(3)
C29	0.086(7)	0.079(7)	0.084(7)	-0.002(6)	-0.004(6)	0.030(6)
C28	0.029(3)	0.044(4)	0.044(4)	0.017(3)	0.005(3)	0.010(3)
C27	0.074(5)	0.045(4)	0.045(4)	0.023(4)	-0.004(4)	-0.014(4)
C26	0.087(6)	0.065(5)	0.051(5)	0.028(4)	-0.007(4)	-0.005(5)
C25	0.067(5)	0.052(5)	0.065(5)	0.035(4)	0.013(4)	0.014(4)
C24	0.109(8)	0.068(6)	0.073(6)	0.044(5)	0.010(6)	0.010(6)
C23	0.135(10)	0.086(8)	0.091(8)	0.063(7)	0.027(7)	0.018(7)
C22	0.145(11)	0.066(7)	0.110(9)	0.055(7)	0.032(8)	0.010(7)
C21	0.110(8)	0.049(5)	0.077(6)	0.034(5)	0.027(6)	0.013(5)
C20	0.049(4)	0.043(4)	0.067(5)	0.025(4)	0.015(4)	0.014(3)
C19	0.038(3)	0.030(3)	0.054(4)	0.016(3)	0.009(3)	0.009(3)
C18	0.037(4)	0.033(3)	0.059(4)	0.013(3)	0.011(3)	0.008(3)
C17	0.029(3)	0.027(3)	0.057(4)	0.003(3)	-0.005(3)	0.010(3)
C16	0.034(4)	0.033(4)	0.091(6)	0.008(4)	-0.003(4)	0.012(3)
C15	0.048(5)	0.039(4)	0.102(7)	0.004(5)	-0.014(5)	0.019(4)
C30	0.027(3)	0.038(3)	0.029(3)	0.007(3)	0.005(2)	0.018(3)
C31	0.026(3)	0.033(3)	0.040(3)	0.008(3)	0.003(3)	0.006(3)
C32	0.036(3)	0.040(4)	0.042(4)	0.013(3)	0.003(3)	0.015(3)
C33	0.041(4)	0.053(4)	0.035(3)	0.010(3)	0.007(3)	0.022(3)
C34	0.059(5)	0.057(5)	0.041(4)	0.022(3)	0.007(3)	0.019(4)
C35	0.071(5)	0.067(5)	0.032(4)	0.017(4)	0.005(3)	0.022(4)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C36	0.064(5)	0.056(5)	0.032(4)	0.003(3)	-0.001(3)	0.021(4)
C37	0.051(4)	0.045(4)	0.035(4)	0.007(3)	0.004(3)	0.015(3)
C38	0.034(3)	0.039(4)	0.037(3)	0.007(3)	0.002(3)	0.016(3)
C39	0.032(3)	0.038(3)	0.031(3)	0.002(3)	-0.003(3)	0.017(3)
C40	0.035(3)	0.031(3)	0.031(3)	0.000(3)	0.000(3)	0.011(3)
C41	0.028(3)	0.030(3)	0.051(4)	-0.002(3)	-0.002(3)	0.011(3)
C42	0.034(3)	0.041(4)	0.050(4)	-0.004(3)	0.000(3)	0.014(3)
C43	0.034(4)	0.033(4)	0.066(5)	-0.005(3)	-0.012(3)	0.012(3)
C57	0.028(3)	0.043(4)	0.040(4)	0.014(3)	0.009(3)	0.014(3)
C56	0.035(3)	0.038(3)	0.039(4)	0.010(3)	0.006(3)	0.009(3)
C55	0.038(4)	0.048(4)	0.038(4)	0.012(3)	0.008(3)	0.000(3)
C54	0.048(4)	0.057(5)	0.045(4)	0.020(4)	0.009(3)	0.007(4)
C53	0.085(6)	0.062(5)	0.055(5)	0.026(4)	0.013(4)	-0.009(5)
C52	0.109(8)	0.075(6)	0.067(6)	0.033(5)	0.022(6)	0.004(6)
C51	0.100(7)	0.052(5)	0.077(6)	0.032(5)	0.025(5)	-0.002(5)
C50	0.065(5)	0.045(4)	0.067(5)	0.020(4)	0.017(4)	-0.003(4)
C49	0.034(3)	0.052(4)	0.055(4)	0.023(4)	0.010(3)	0.012(3)
C48	0.030(3)	0.033(3)	0.040(4)	0.005(3)	0.006(3)	0.007(3)
C47	0.028(3)	0.039(4)	0.058(4)	0.013(3)	0.007(3)	0.010(3)
C46	0.029(3)	0.033(3)	0.047(4)	0.005(3)	0.009(3)	0.012(3)
C45	0.041(4)	0.037(4)	0.062(5)	0.008(3)	0.010(3)	0.009(3)
C44	0.043(4)	0.036(4)	0.066(5)	0.011(4)	0.010(4)	0.009(3)
C58	0.058(5)	0.051(5)	0.061(5)	0.011(4)	0.009(4)	0.016(4)
C59	0.028(3)	0.040(4)	0.039(4)	-0.004(3)	0.005(3)	0.014(3)
C60	0.032(3)	0.051(4)	0.037(4)	-0.003(3)	0.000(3)	0.010(3)
C61	0.032(3)	0.054(4)	0.049(4)	0.011(3)	0.004(3)	0.007(3)
C62	0.028(3)	0.048(4)	0.058(4)	0.012(3)	0.002(3)	0.012(3)
C63	0.045(4)	0.053(5)	0.065(5)	0.018(4)	-0.005(4)	0.008(4)
C64	0.050(4)	0.043(4)	0.080(6)	0.026(4)	-0.004(4)	0.005(4)
C65	0.045(4)	0.048(5)	0.074(6)	0.005(4)	-0.013(4)	0.010(4)
C66	0.035(4)	0.038(4)	0.064(5)	0.004(3)	0.001(3)	0.008(3)
C67	0.030(3)	0.047(4)	0.052(4)	0.008(3)	0.002(3)	0.012(3)
C68	0.027(3)	0.035(3)	0.048(4)	0.001(3)	0.003(3)	0.008(3)
C69	0.029(3)	0.037(4)	0.048(4)	-0.008(3)	-0.005(3)	0.013(3)
C70	0.034(4)	0.061(5)	0.036(4)	-0.004(3)	-0.005(3)	0.026(3)
C71	0.058(5)	0.057(5)	0.049(4)	-0.010(4)	-0.011(4)	0.027(4)
C72	0.074(6)	0.081(6)	0.032(4)	-0.025(4)	-0.021(4)	0.047(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C73	0.096(7)	0.071(6)	0.046(5)	0.004(4)	0.001(5)	0.044(6)
C74	0.074(5)	0.077(6)	0.034(4)	0.008(4)	0.006(4)	0.047(5)
C75	0.049(4)	0.070(5)	0.037(4)	0.007(4)	0.005(3)	0.037(4)
C76	0.045(4)	0.063(5)	0.046(4)	0.027(4)	0.013(3)	0.034(4)
C77	0.038(4)	0.052(4)	0.038(4)	0.010(3)	0.008(3)	0.025(3)
C78	0.045(4)	0.068(5)	0.054(4)	0.033(4)	0.022(3)	0.030(4)
C79	0.056(5)	0.089(6)	0.050(4)	0.030(4)	0.014(4)	0.030(4)
C80	0.066(5)	0.124(9)	0.060(5)	0.059(6)	0.026(5)	0.038(6)
C81	0.093(7)	0.089(7)	0.071(6)	0.045(6)	0.025(6)	0.019(6)
C82	0.108(8)	0.065(6)	0.076(6)	0.037(5)	0.025(6)	0.020(5)
C83	0.078(6)	0.051(4)	0.053(5)	0.023(4)	0.025(4)	0.027(4)
C84	0.095(7)	0.047(5)	0.052(5)	0.014(4)	0.023(5)	0.013(4)
C85	0.076(5)	0.043(4)	0.041(4)	0.011(3)	0.017(4)	0.021(4)
C86	0.046(4)	0.036(4)	0.048(4)	0.016(3)	0.018(3)	0.020(3)

Table S18. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for $[Er_2(L\text{-}CN)_3]$.

	x/a	y/b	z/c	U(eq)
H7WA	0.224(8)	0.504(6)	0.529(5)	0.11(4)
H7WB	0.106(12)	0.49(3)	0.515(13)	0.9(5)
H2	-0.1892	0.4726	0.6658	0.058
H3	-0.2488	0.4564	0.7754	0.064
H5	-0.2260	0.5043	0.9141	0.064
H6	-0.1420	0.6050	1.0276	0.066
H7	0.0032	0.7234	1.0324	0.066
H8	0.0552	0.7466	0.9244	0.057
H11	0.0567	0.7659	0.8235	0.05
H13	0.2011	0.8697	0.8555	0.068
H27	-0.0482	0.5630	0.3685	0.072
H26	-0.0437	0.6162	0.2759	0.087
H24	0.0309	0.7258	0.2298	0.099
H23	0.1420	0.8554	0.2520	0.118
H22	0.2508	0.9349	0.3726	0.125
H21	0.2525	0.8870	0.4717	0.093
H18	0.1876	0.8485	0.5535	0.053
H16	0.3177	0.9273	0.6421	0.067

	x/a	y/b	z/c	U(eq)
H15	0.3792	1.0265	0.7586	0.082
H31	0.1784	0.5217	0.7340	0.041
H32	0.1381	0.4965	0.8431	0.047
H34	0.1627	0.5398	0.9813	0.061
H35	0.2531	0.6360	1.0973	0.068
H36	0.3826	0.7599	1.1048	0.064
H37	0.4233	0.7890	0.9970	0.054
H40	0.4076	0.8172	0.8973	0.042
H42	0.5737	0.9191	0.9327	0.055
H56	0.3225	0.5980	0.4559	0.046
H55	0.3634	0.6372	0.3559	0.053
H53	0.4515	0.7393	0.3011	0.087
H52	0.5696	0.8669	0.3178	0.103
H51	0.6500	0.9577	0.4371	0.094
H50	0.6205	0.9223	0.5422	0.075
H47	0.5436	0.8914	0.6296	0.051
H45	0.6947	0.9711	0.7174	0.059
H44	0.7628	1.0711	0.8322	0.061
H60	0.7464	0.6995	0.4978	0.054
H61	0.8726	0.8041	0.4718	0.057
H63	1.0146	0.9413	0.5141	0.068
H64	1.1160	1.0596	0.6091	0.071
H65	1.0961	1.0718	0.7324	0.074
H66	0.9804	0.9651	0.7643	0.059
H69	0.9185	0.8609	0.7847	0.052
H71	0.9134	0.8946	0.8966	0.073
H73	0.7547	0.8034	1.0522	0.086
H74	0.6228	0.6935	0.9562	0.071
H76	0.6108	0.5931	0.8681	0.054
H79	0.5026	0.5125	0.9087	0.074
H80	0.4177	0.4054	0.9457	0.088
H81	0.2972	0.2846	0.8584	0.097
H82	0.2590	0.2725	0.7337	0.096
H84	0.2921	0.3260	0.6313	0.08
H85	0.3720	0.4268	0.5889	0.063

Table S19. Hydrogen bond distances (Å) and angles (°) for [Er_2(L-CN)$_3$].

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O7W-H7WB···O5#1	0.84(2)	2.3(5)	2.904(6)	130.(50)
C13-H13···N6#2	0.95	2.3	3.186(12)	154.6
C27-H27···O7W#1	0.95	2.62	3.336(8)	132.8
C42-H42···N3#2	0.95	2.38	3.281(13)	157.3
C71-H71···N9#3	0.95	2.31	3.215(14)	158.2

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y+1, -z+1

#2 -x+1, -y+2, -z+2

#3 -x+2, -y+2, -z+2

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