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Construction of three unusual tetranuclear lanthanide complexes based on salicylate and phenanthroline ligands

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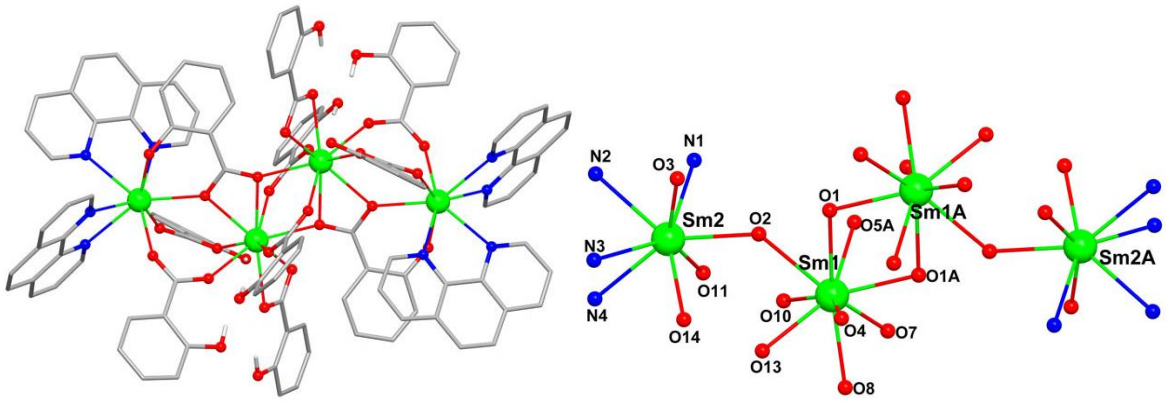
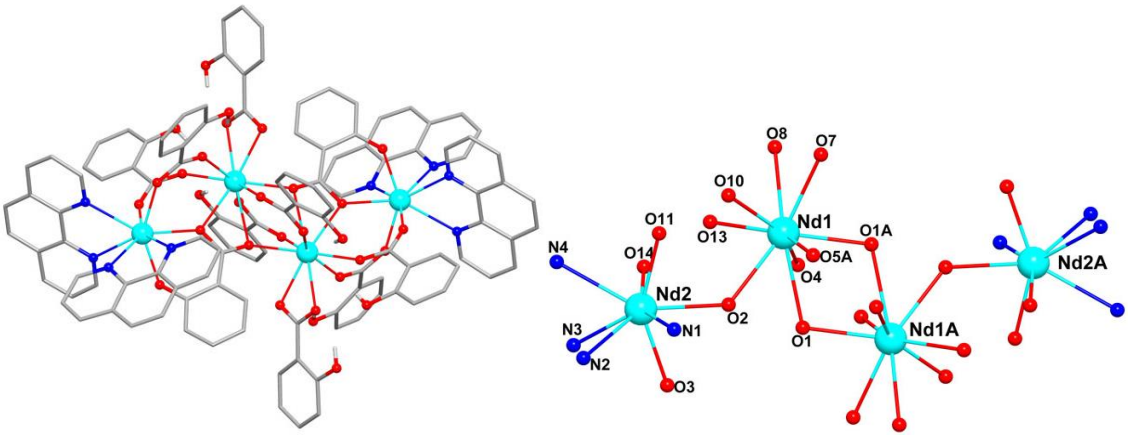
Figures:

Tables:



(a) (b)

Figure S1 (a) Molecular structure of **2** and (b) Local coordination environment of Sm^{III} in **2** (symmetry codes for A = –*x* + 1, –*y* + 1, –*z* + 2) .



(a) (b)

Figure S2 (a) Molecular structure of **3** and (b) Local coordination environment of Nd^{III} in **3** (symmetry codes for A = –*x* + 1, –*y* + 1, –*z* + 2) .

Table S1 Crystallographic data and structure refinement summary for **1**–**3**.[a]

	1	**2**	**3**
Chemical formula	$C_{59}H_{40}Eu_2N_4O_{15}$	$C_{59}H_{40}N_4O_{15}Sm_2$	$C_{59}H_{40}N_4Nd_2O_{15}$
Formula Mass	1348.87	1345.65	1333.43
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*P2(1)/c*	*P2(1)/c*	*P2(1)/c*
a/Å	16.6472(4)	16.6472(4)	16.6472(4)
b/Å	20.7052(5)	20.7052(5)	20.7052(5)
c/Å	16.0879(5)	16.0879(5)	16.0879(5)
β/°	106.283	106.283	106.283
V/Å^3	5322.8(2)	5322.8(2)	5322.8(2)
T/K	293(2)	293(2)	293(2)
Z	4	4	4
μ/mm^{-1}	2.410	2.260	2.004
R_{int}	0.0454	0.0314	0.0480
[a]R_1 ($I > 2\sigma(I)$)	0.0258	0.0246	0.0266
[b]wR_2 (all data)	0.0361	0.0407	0.0325
GOF	0.974	0.834	0.932
$\Delta\rho_{max,\ min}$ /e·Å^{-3}	0.651, –0.517	0.460, –0.429	0.706, –0.517

[a] $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$; [b] $wR_2 = [\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond lengths (Å) and angles (°) for complex **1**[a].

Eu(1)–O(10)	2.398(2)	Eu(1)–O(4)	2.425(2)
Eu(1)–O(13)	2.427(2)	Eu(1)–O(7)	2.510(2)
Eu(1)–O(8)	2.511(2)	Eu(1)–O(2)	2.5248(19)
Eu(1)–O(1)	2.625(2)	Eu(2)–O(3)	2.204(2)
Eu(2)–O(11)	2.321(2)	Eu(2)–O(14)	2.334(2)
Eu(2)–O(2)	2.422(2)	Eu(2)–N(3)	2.599(3)
Eu(2)–N(4)	2.610(3)	Eu(2)–N(1)	2.631(3)
Eu(2)–N(2)	2.640(3)		
$O(5)^{\#1}$–Eu(1)–O(10)	73.88(8)	O(10)–Eu(1)–$O(1)^{\#1}$	138.36(7)
$O(5)^{\#1}$–Eu(1)–O(4)	134.19(7)	O(10)–Eu(1)–O(4)	148.52(8)
$O(1)^{\#1}$–Eu(1)–O(4)	71.79(7)	$O(5)^{\#1}$–Eu(1)–O(13)	144.89(8)
O(10)–Eu(1)–O(13)	78.57(8)	$O(1)^{\#1}$–Eu(1)–O(13)	138.73(7)
O(4)–Eu(1)–O(13)	69.96(8)	$O(5)^{\#1}$–Eu(1)–O(7)	75.79(7)
O(10)–Eu(1)–O(7)	70.62(7)	$O(1)^{\#1}$–Eu(1)–O(7)	75.05(7)
O(4)–Eu(1)–O(7)	123.55(7)	O(13)–Eu(1)–O(7)	114.88(7)
$O(5)^{\#1}$–Eu(1)–O(8)	126.44(7)	O(10)–Eu(1)–O(8)	78.13(7)
$O(1)^{\#1}$–Eu(1)–O(8)	98.68(7)	O(4)–Eu(1)–O(8)	89.85(7)
O(13)–Eu(1)–O(8)	66.58(7)	O(7)–Eu(1)–O(8)	51.95(7)
$O(5)^{\#1}$–Eu(1)–O(2)	77.03(7)	O(10)–Eu(1)–O(2)	77.77(7)
$O(1)^{\#1}$–Eu(1)–O(2)	121.37(7)	O(4)–Eu(1)–O(2)	93.63(7)
O(13)–Eu(1)–O(2)	76.20(7)	O(7)–Eu(1)–O(2)	142.80(7)
O(8)–Eu(1)–O(2)	138.80(7)	$O(5)^{\#1}$–Eu(1)–O(1)	67.63(7)
O(10)–Eu(1)–O(1)	119.91(7)	$O(1)^{\#1}$–Eu(1)–O(1)	71.50(7)
O(4)–Eu(1)–O(1)	72.11(7)	O(13)–Eu(1)–O(1)	109.93(7)
O(7)–Eu(1)–O(1)	135.19(7)	O(8)–Eu(1)–O(1)	161.30(7)
O(2)–Eu(1)–O(1)	50.24(7)	O(3)–Eu(2)–O(11)	144.16(8)
O(3)–Eu(2)–O(14)	109.49(8)	O(11)–Eu(2)–O(14)	86.58(7)
O(3)–Eu(2)–O(2)	73.54(7)	O(11)–Eu(2)–O(2)	79.12(8)
O(14)–Eu(2)–O(2)	78.17(7)	O(3)–Eu(2)–N(3)	77.94(9)
O(11)–Eu(2)–N(3)	137.83(9)	O(14)–Eu(2)–N(3)	70.96(8)
O(2)–Eu(2)–N(3)	127.33(8)	O(3)–Eu(2)–N(4)	137.31(8)
O(11)–Eu(2)–N(4)	77.06(8)	O(14)–Eu(2)–N(4)	74.48(8)

O(2)–Eu(2)–N(4)	144.48(7)	N(3)–Eu(2)–N(4)	62.95(9)
O(3)–Eu(2)–N(1)	79.21(8)	O(11)–Eu(2)–N(1)	73.42(8)
O(14)–Eu(2)–N(1)	152.58(8)	O(2)–Eu(2)–N(1)	79.73(8)
N(3)–Eu(2)–N(1)	136.24(8)	N(4)–Eu(2)–N(1)	117.41(9)
O(3)–Eu(2)–N(2)	78.53(9)	O(11)–Eu(2)–N(2)	107.54(8)
O(14)–Eu(2)–N(2)	143.90(9)	O(2)–Eu(2)–N(2)	136.26(8)
N(3)–Eu(2)–N(2)	76.87(9)	N(4)–Eu(2)–N(2)	76.63(9)
N(1)–Eu(2)–N(2)	62.27(9)		

Symmetry codes for **1**: #1 –x + 1, –y + 1, –z + 2

Table S3 Selected bond lengths (Å) and angles (°) for complex **2**[a].

Sm(1)–O(10)	2.413(2)	Sm(1)–O(13)	2.4289(19)
Sm(1)–O(4)	2.436(2)	Sm(1)–O(7)	2.513(2)
Sm(1)–O(8)	2.522(2)	Sm(1)–O(2)	2.534(2)
Sm(1)–O(1)	2.6329(19)	Sm(2)–O(3)	2.209(2)
Sm(2)–O(11)	2.334(2)	Sm(2)–O(14)	2.353(2)
Sm(2)–O(2)	2.4254(19)	Sm(2)–N(3)	2.610(3)
Sm(2)–N(4)	2.626(2)	Sm(2)–N(1)	2.643(3)
Sm(2)–N(2)	2.646(3)		
O(5)$^{\#1}$–Sm(1)–O(10)	73.74(7)	O(10)–Sm(1)–O(1)$^{\#1}$	138.12(7)
O(5)$^{\#1}$–Sm(1)–O(13)	144.96(8)	O(10)–Sm(1)–O(13)	79.02(7)
O(1)$^{\#1}$–Sm(1)–O(13)	138.66(7)	O(5)$^{\#1}$–Sm(1)–O(4)	133.98(7)
O(10)–Sm(1)–O(4)	148.84(7)	O(1)$^{\#1}$–Sm(1)–O(4)	71.77(7)
O(13)–Sm(1)–O(4)	69.83(7)	O(5)$^{\#1}$–Sm(1)–O(7)	76.30(7)
O(10)–Sm(1)–O(7)	70.39(7)	O(1)$^{\#1}$–Sm(1)–O(7)	75.37(7)
O(13)–Sm(1)–O(7)	114.66(7)	O(4)–Sm(1)–O(7)	123.47(7)
O(5)$^{\#1}$–Sm(1)–O(8)	126.47(7)	O(10)–Sm(1)–O(8)	78.01(7)
O(1)$^{\#1}$–Sm(1)–O(8)	98.95(7)	O(13)–Sm(1)–O(8)	66.70(7)
O(4)–Sm(1)–O(8)	90.13(7)	O(7)–Sm(1)–O(8)	51.48(7)
O(5)$^{\#1}$–Sm(1)–O(2)	76.81(7)	O(10)–Sm(1)–O(2)	77.81(7)
O(1)$^{\#1}$–Sm(1)–O(2)	121.21(6)	O(13)–Sm(1)–O(2)	76.23(6)
O(4)–Sm(1)–O(2)	93.66(7)	O(7)–Sm(1)–O(2)	142.87(7)
O(8)–Sm(1)–O(2)	138.76(6)	O(5)$^{\#1}$–Sm(1)–O(1)	67.51(7)
O(10)–Sm(1)–O(1)	119.63(7)	O(1)$^{\#1}$–Sm(1)–O(1)	71.68(8)
O(13)–Sm(1)–O(1)	109.54(7)	O(4)–Sm(1)–O(1)	72.10(7)
O(7)–Sm(1)–O(1)	135.80(6)	O(8)–Sm(1)–O(1)	161.66(7)
O(2)–Sm(1)–O(1)	49.91(6)	O(3)–Sm(2)–O(11)	143.99(7)
O(3)–Sm(2)–O(14)	109.62(8)	O(11)–Sm(2)–O(14)	86.42(8)
O(3)–Sm(2)–O(2)	73.26(7)	O(11)–Sm(2)–O(2)	79.28(7)
O(14)–Sm(2)–O(2)	78.03(7)	O(3)–Sm(2)–N(3)	77.98(8)
O(11)–Sm(2)–N(3)	137.97(8)	O(14)–Sm(2)–N(3)	71.26(8)
O(2)–Sm(2)–N(3)	127.17(8)	O(3)–Sm(2)–N(4)	137.40(8)
O(11)–Sm(2)–N(4)	77.15(8)	O(14)–Sm(2)–N(4)	74.46(8)

O(2)–Sm(2)–N(4)	144.57(7)	N(3)–Sm(2)–N(4)	62.95(9)
O(3)–Sm(2)–N(1)	79.27(8)	O(11)–Sm(2)–N(1)	73.37(8)
O(14)–Sm(2)–N(1)	152.57(8)	O(2)–Sm(2)–N(1)	80.08(8)
N(3)–Sm(2)–N(1)	135.99(9)	N(4)–Sm(2)–N(1)	117.22(9)
O(3)–Sm(2)–N(2)	78.74(8)	O(11)–Sm(2)–N(2)	107.33(9)
O(14)–Sm(2)–N(2)	144.16(8)	O(2)–Sm(2)–N(2)	136.21(7)
N(3)–Sm(2)–N(2)	76.96(8)	N(4)–Sm(2)–N(2)	76.63(8)
N(1)–Sm(2)–N(2)	61.90(8)		

Symmetry transformations used to generate equivalent atoms: #1 –x + 1, –y + 1, –z + 2

Table S4 Selected bond lengths (Å) and angles (°) for complex **3**[a].

Nd(1)–O(10)	2.4329(19)	Nd(1)–O(13)	2.449(2)
Nd(1)–O(4)	2.465(2)	Nd(1)–O(7)	2.529(2)
Nd(1)–O(8)	2.536(2)	Nd(1)–O(2)	2.5552(19)
Nd(1)–O(1)	2.6461(19)	Nd(2)–O(3)	2.224(2)
Nd(2)–O(11)	2.362(2)	Nd(2)–O(14)	2.379(2)
Nd(2)–O(2)	2.431(2)	Nd(2)–N(3)	2.623(3)
Nd(2)–N(4)	2.637(3)	Nd(2)–N(2)	2.663(3)
Nd(2)–N(1)	2.669(3)		
$O(5)^{\#1}$–Nd(1)–O(10)	73.40(7)	$O(5)^{\#1}$–Nd(1)–$O(1)^{\#1}$	75.25(7)
O(10)–Nd(1)–$O(1)^{\#1}$	137.84(7)	$O(5)^{\#1}$–Nd(1)–O(13)	144.86(7)
O(10)–Nd(1)–O(13)	79.41(7)	$O(1)^{\#1}$–Nd(1)–O(13)	138.77(7)
$O(5)^{\#1}$–Nd(1)–O(4)	133.83(7)	O(10)–Nd(1)–O(4)	149.24(7)
$O(1)^{\#1}$–Nd(1)–O(4)	71.76(7)	O(13)–Nd(1)–O(4)	69.84(7)
$O(5)^{\#1}$–Nd(1)–O(7)	76.61(7)	O(10)–Nd(1)–O(7)	70.30(7)
$O(1)^{\#1}$–Nd(1)–O(7)	75.57(7)	O(13)–Nd(1)–O(7)	114.62(7)
O(4)–Nd(1)–O(7)	123.42(7)	$O(5)^{\#1}$–Nd(1)–O(8)	126.68(7)
O(10)–Nd(1)–O(8)	78.05(7)	$O(1)^{\#1}$–Nd(1)–O(8)	99.44(7)
O(13)–Nd(1)–O(8)	66.59(7)	O(4)–Nd(1)–O(8)	90.28(7)
O(7)–Nd(1)–O(8)	51.45(7)	$O(5)^{\#1}$–Nd(1)–O(2)	76.40(7)
O(10)–Nd(1)–O(2)	77.73(7)	$O(1)^{\#1}$–Nd(1)–O(2)	120.84(7)
O(13)–Nd(1)–O(2)	76.41(7)	O(4)–Nd(1)–O(2)	93.79(6)
O(7)–Nd(1)–O(2)	142.78(6)	O(8)–Nd(1)–O(2)	138.70(7)
$O(5)^{\#1}$–Nd(1)–O(1)	67.50(7)	O(10)–Nd(1)–O(1)	119.14(7)
$O(1)^{\#1}$–Nd(1)–O(1)	71.93(7)	O(13)–Nd(1)–O(1)	109.08(7)
O(4)–Nd(1)–O(1)	72.08(6)	O(7)–Nd(1)–O(1)	136.30(7)
O(8)–Nd(1)–O(1)	161.96(6)	O(2)–Nd(1)–O(1)	49.35(6)
O(3)–Nd(2)–O(11)	143.89(8)	O(3)–Nd(2)–O(14)	109.37(8)
O(11)–Nd(2)–O(14)	86.82(7)	O(3)–Nd(2)–O(2)	72.86(7)
O(11)–Nd(2)–O(2)	79.63(7)	O(14)–Nd(2)–O(2)	78.20(7)
O(3)–Nd(2)–N(3)	78.21(9)	O(11)–Nd(2)–N(3)	137.86(9)
O(14)–Nd(2)–N(3)	71.32(8)	O(2)–Nd(2)–N(3)	127.41(7)
O(3)–Nd(2)–N(4)	136.92(8)	O(11)–Nd(2)–N(4)	77.75(9)

O(14)–Nd(2)–N(4)	74.44(8)	O(2)–Nd(2)–N(4)	145.17(8)
N(3)–Nd(2)–N(4)	62.08(9)	O(3)–Nd(2)–N(2)	78.50(8)
O(11)–Nd(2)–N(2)	106.86(8)	O(14)–Nd(2)–N(2)	145.07(9)
O(2)–Nd(2)–N(2)	135.08(8)	N(3)–Nd(2)–N(2)	77.52(9)
N(4)–Nd(2)–N(2)	77.31(9)	O(3)–Nd(2)–N(1)	79.09(8)
O(11)–Nd(2)–N(1)	73.39(8)	O(14)–Nd(2)–N(1)	152.80(9)
O(2)–Nd(2)–N(1)	79.99(8)	N(3)–Nd(2)–N(1)	135.68(9)
N(4)–Nd(2)–N(1)	117.69(8)	N(2)–Nd(2)–N(1)	60.90(9)

Symmetry transformations used to generate equivalent atoms: #1 –x + 1, –y + 1, –z + 2

Table S5 Hydrogen bond lengths (Å) and angles (°) for complex **1**[a]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
C52–H52A···O9[a]	0.93	2.467	3.337(5)	156

[a]Symmetry codes for **1**: a = –*x*, *y* – 1/2, –*z* + 3/2.