Supporting Information for

Two chiral Eu^{III} and Sm^{III} enantiomeric pairs with enantiopure N-donor ligands: showing strong third-harmonic generation and photoluminescence properties

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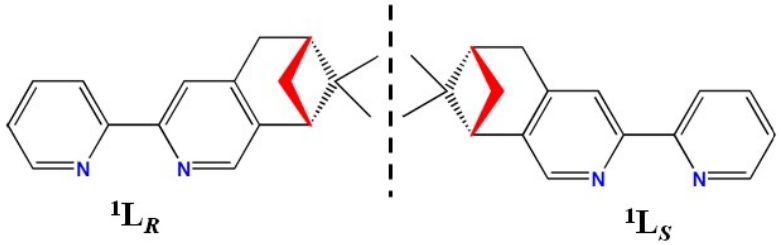

Scheme S1. Chemical structures of enantiopure bidentate N-donors ^1L_R and ^1L_S.

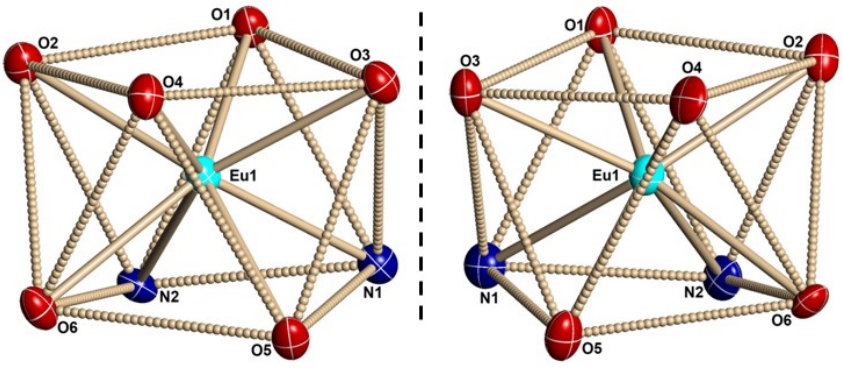

Fig. S1. Coordination geometries of Eu1 in **D-1**(left) and **L-1** (right).

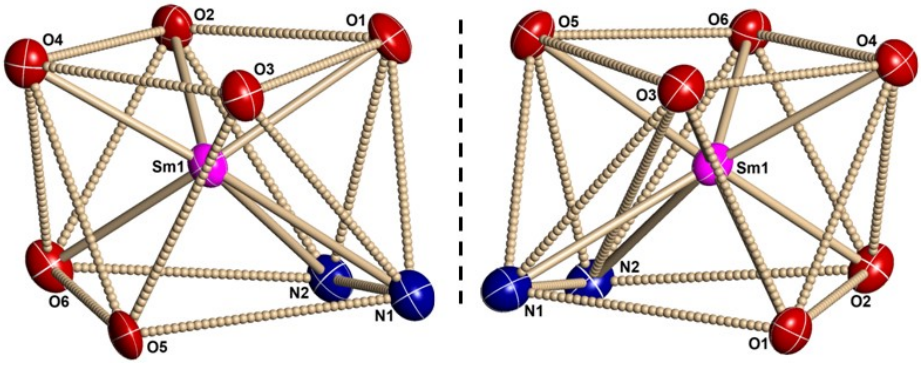

Fig. S2. Coordination geometries of Sm1 in **D-2**(left) and **L-2** (right).

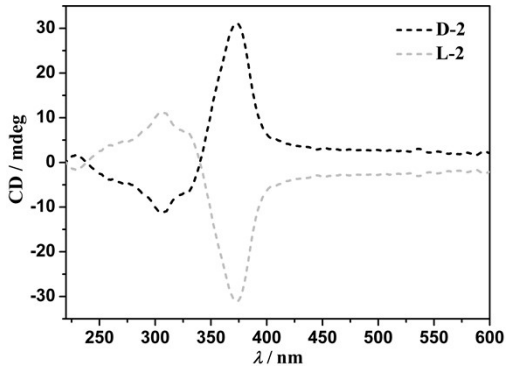

Fig. S3. Solid-state CD spectra of **D-2**/**L-2** enantiomeric pairs at room temperature.

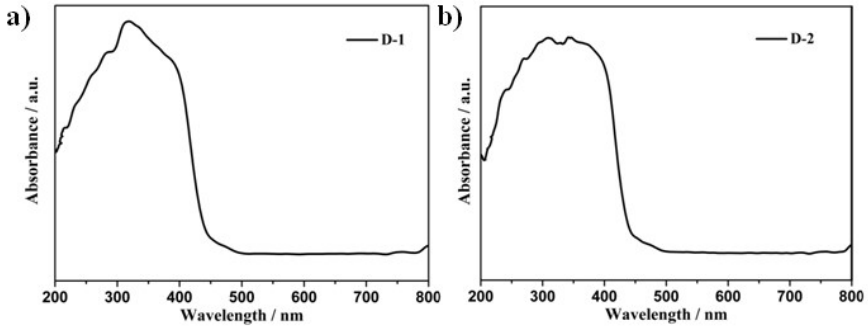

Fig. S4. UV-vis diffuse reflectance spectra of **D-1** (a) and **D-2** (b).

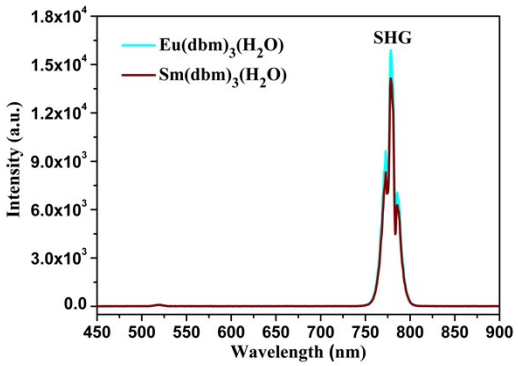

Fig. S5. SHG spectra of $Eu(dbm)_3(H_2O)$ and $Sm(dbm)_3(H_2O)$ under excitation at λ = 1550 nm (T_{int} = 0.5 s).

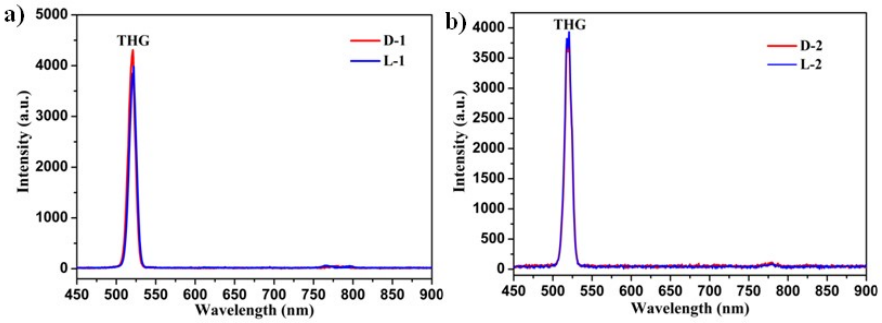

Fig. S6. THG spectra of **D-1/L-1** (a) and **D-2/L-2** (b) under excitation at λ = 1550 nm (T_{int} = 0.5 s).

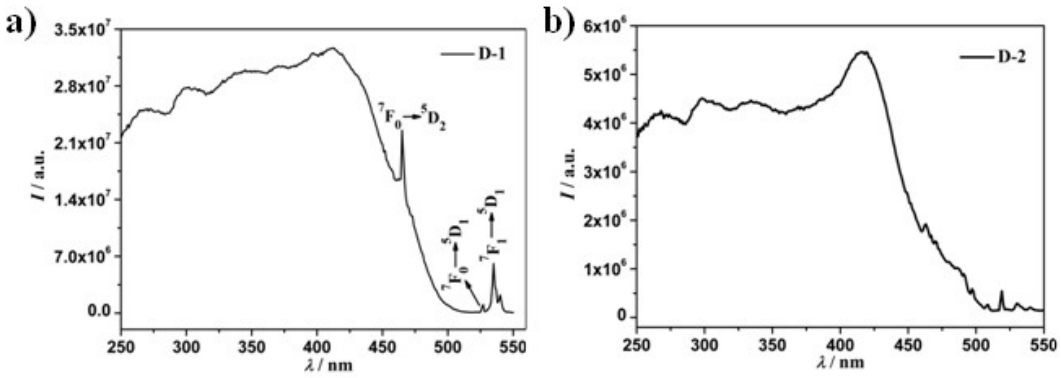

Fig. S7. Solid-state excitation spectra of **D-1** (a, λ_{em} = 613 nm) and **D-2** (b, λ_{em} = 648 nm) at room temperature.

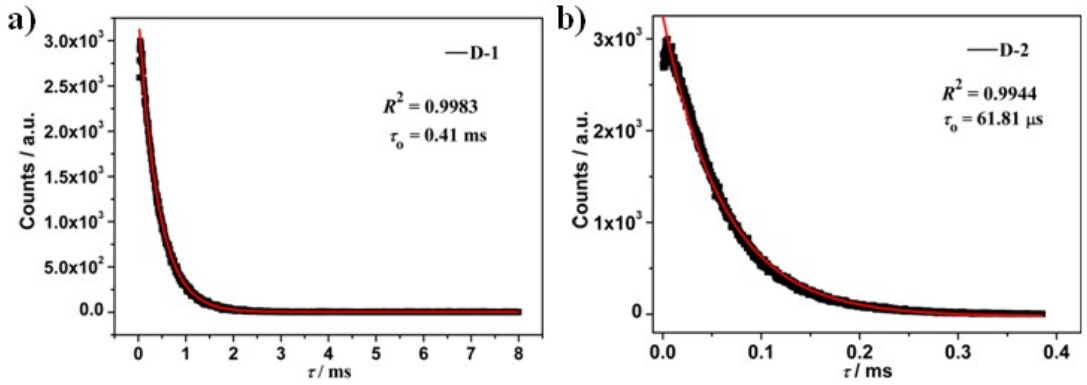

Fig. S8. Decay curves of **D-1** (a) and **D-2** (b) with the corresponding fitted curves (red) in the solid state at room temperature.

Table S1 Crystallographic data and structure refinement parameters for **D-1/L-1** and **D-2/L-2** enantiomeric pairs.

Complex	**D-1**	**L-1**	**D-2**	**L-2**
Chemical formula	$C_{61}H_{50}N_2O_3Eu$	$C_{61}H_{50}N_2O_3Eu$	$C_{61}H_{50}N_2O_3Sm$	$C_{61}H_{50}N_2O_3Sm$
Formula weight	1073.00	1073.00	1071.39	1071.39
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a (Å)	9.5427(2)	9.5536(9)	9.5520(2)	9.5481(2)
b (Å)	20.9229(5)	20.8906(12)	20.9501(5)	20.9561(4)
c (Å)	12.6458(4)	12.6394(10)	12.6405(3)	12.6388(4)
β (deg)	93.541(3)	93.363(9)	93.560(2)	93.576(2)
V(Å^3)	2520.05(11)	2518.20(3)	2524.68(10)	2523.99(11)
Z	2	2	2	2
D_c(g cm^{-3})	1.414	1.415	1.409	1.410
μ (mm^{-1})	1.300	1.301	9.178	9.181
F(000)	1096	1096	1094	1094
Reflections collected	11500	10443	9639	9671
Independent reflections	8224	7084	6581	6743
Data/restraints/parameters	8224/1/642	7084/1394/642	6581/4/642	6743/1/642
GOF	1.015	1.048	1.062	1.057
R_1 [$I >= 2\sigma$ (I)][a]	0.0353	0.0824	0.0833	0.0491
wR_2 [$I >= 2\sigma$ (I)][b]	0.0639	0.1527	0.2166	0.1275
Flack parameter	0.020(8)	0.01(2)	0.006(8)	0.014(5)
CCDC	2382191	2382192	2382193	2382326

[a] $R_1 = \sum||Fo|-|Fc||/\sum|Fo|$. [b] $_wR_2 = [\sum w(Fo^2 - Fc^2)^2/\sum w(Fo^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) and angles (°) for **D-1** and **L-1**.

Bond lengths for **D-1**					
Eu(1)─O(1)	2.372(6)	Eu(1)─O(2)	2.341(6)	Eu(1)─O(3)	2.362(4)
Eu(1)─O(4)	2.347(4)	Eu(1)─O(5)	2.373(6)	Eu(1)─O(6)	2.362(5)
Eu(1)─N(1)	2.652(5)	Eu(1)─N(2)	2.610(5)		
Bond lengths for **L-1**					
Eu(1)─O(1)	2.392(15)	Eu(1)─O(2)	2.339(14)	Eu(1)─O(3)	2.347(10)
Eu(1)─O(4)	2.362(13)	Eu(1)─O(5)	2.330(17)	Eu(1)─O(6)	2.371(13)
Eu(1)─N(1)	2.655(14)	Eu(1)─N(2)	2.584(16)		
Bond angles for **D-1**					
O(3)-Eu(1)-O(2)	123.6(2)	O(3)-Eu(1)-O(5)	76.5(3)	O(6)-Eu(1)-O(5)	72.8(2)
O(1)-Eu(1)-O(3)	80.5(3)	O(6)-Eu(1)-N(1)	118.4(2)	O(3)-Eu(1)-N(2)	139.13(17)
Bond angles for **L-1**					
O(3)-Eu(1)-O(2)	123.3(6)	O(3)-Eu(1)-O(5)	76.3(7)	O(6)-Eu(1)-O(5)	72.0(6)
O(1)-Eu(1)-O(3)	80.7(6)	O(6)-Eu(1)-N(1)	118.6(6)	O(3)-Eu(1)-N(2)	139.0(5)

Table S3 Selected bond lengths (Å) and angles (°) for **D-2** and **L-2**.

Bond lengths for **D-2**					
Sm(1)─O(1)	2.398(12)	Sm(1)─O(2)	2.342(10)	Sm(1)─O(3)	2.384(8)
Sm(1)─O(4)	2.335(10)	Sm(1)─O(5)	2.390(12)	Sm(1)─O(6)	2.379(10)
Sm(1)─N(1)	2.658(13)	Sm(1)─N(2)	2.628(12)		
Bond lengths for **L-2**					
Sm(1)─O(1)	2.376(8)	Sm(1)─O(2)	2.372(7)	Sm(1)─O(3)	2.363(5)
Sm(1)─O(4)	2.346(6)	Sm(1)─O(5)	2.394(8)	Sm(1)─O(6)	2.344(7)
Sm(1)─N(1)	2.653(8)	Sm(1)─N(2)	2.622(7)		
Bond angles for **D-2**					
O(3)-Sm(1)-O(2)	123.0(5)	O(3)-Sm(1)-O(5)	77.8(5)	O(6)-Sm(1)-O(5)	71.6(4)
O(1)-Sm(1)-O(3)	79.9(5)	O(6)-Sm(1)-N(1)	118.1(5)	O(3)-Sm(1)-N(2)	138.9(4)
Bond angles for **L-2**					
O(3)-Sm(1)-O(2)	138.3(3)	O(3)-Sm(1)-O(5)	81.0(3)	O(6)-Sm(1)-O(5)	70.4(3)
O(1)-Sm(1)-O(3)	77.2(3)	O(6)-Sm(1)-N(1)	129.2(3)	O(3)-Sm(1)-N(2)	139.5(2)

Table S4 Continuous shape measures calculation for Eu1 in **D-1**. The lowest CShMs value is highlighted.

OP-8	1 D_{8h}	Octagon
HPY-8	2 C_{7v}	Heptagonal pyramid
HBPY-8	3 D_{6h}	Hexagonal bipyramid
CU-8	4 O_h	Cube
SAPR-8	5 D_{4d}	Square antiprism
TDD-8	6 D_{2d}	Triangular dodecahedron
JGBF-8	7 D_{2d}	Johnson gyrobifastigium J26
JETBPY-8	8 D_{3h}	Johnson elongated triangular bipyramid J14
JBTPR-8	9 C_{2v}	Biaugmented trigonal prism J50
BTPR-8	10 C_{2v}	Biaugmented trigonal prism
JSD-8	11 D_{2d}	Snub diphenoid J84
TT-8	12 T_d	Triakis tetrahedron
ETBPY-8	13 D_{3h}	Elongated trigonal bipyrami

Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	31.014,	23.057,	13.813,	6.556,	**0.973**,	1.826,	15.819,	28.192,	3.361,	2.777,	5.384,	7.330,	23.549

Table S5 Continuous shape measures calculation for Eu1 in **L-1**. The lowest CShMs value is highlighted.

OP-8	1 D_{8h}	Octagon
HPY-8	2 C_{7v}	Heptagonal pyramid
HBPY-8	3 D_{6h}	Hexagonal bipyramid
CU-8	4 O_h	Cube
SAPR-8	5 D_{4d}	Square antiprism
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Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	31.034,	22.821,	13.844,	6.679,	**0.974**,	1.902,	15.857,	28.260,	3.345,	2.827,	5.411,	7.452,	23.419

Table S6 Continuous shape measures calculation for Sm1 in **D-2**. The lowest CShMs value is highlighted.

OP-8	1 D_{8h}	Octagon
HPY-8	2 C_{7v}	Heptagonal pyramid
HBPY-8	3 D_{6h}	Hexagonal bipyramid
CU-8	4 O_h	Cube
SAPR-8	5 D_{4d}	Square antiprism
TDD-8	6 D_{2d}	Triangular dodecahedron
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TT-8	12 T_d	Triakis tetrahedron
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Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY	29.099,	22.734,	16.541,	10.102,	**0.776**,	1.722,	15.182,	27.602,	2.333,	1.824,	4.386,	10.749,	23.073

Table S7 Continuous shape measures calculation for Sm1 in **L-2**. The lowest CShMs value is highlighted.

OP-8	1 D_{8h}	Octagon
HPY-8	2 C_{7v}	Heptagonal pyramid
HBPY-8	3 D_{6h}	Hexagonal bipyramid
CU-8	4 O_h	Cube
SAPR-8	5 D_{4d}	Square antiprism
TDD-8	6 D_{2d}	Triangular dodecahedron
JGBF-8	7 D_{2d}	Johnson gyrobifastigium J26
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Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY	28.955,	22.469,	16.467,	10.117,	**0.828**,	1.719,	15.176,	27.377,	2.298,	1.793,	4.395,	10.771,	22.892