Supporting information for

Two chiral lanthanide Pr^{III} and Ho^{III} complexes: NIR luminescent and nonlinear optical properties

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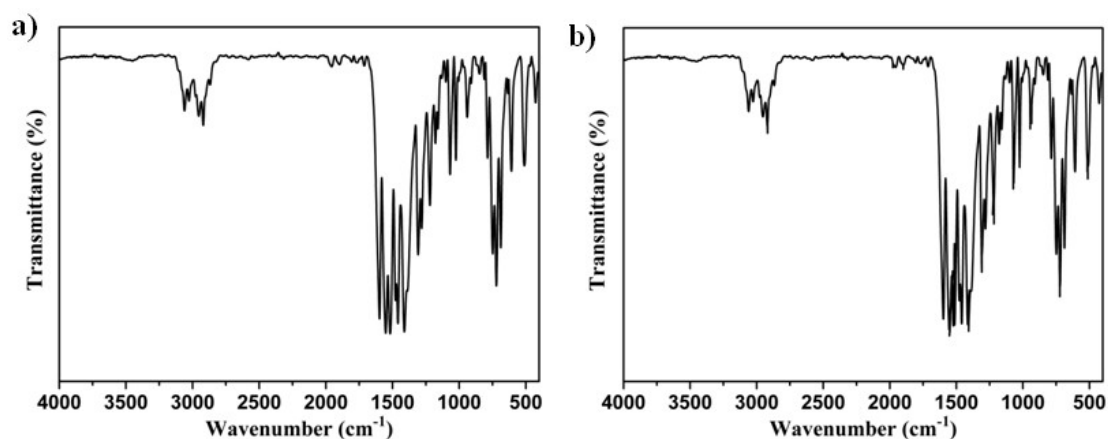
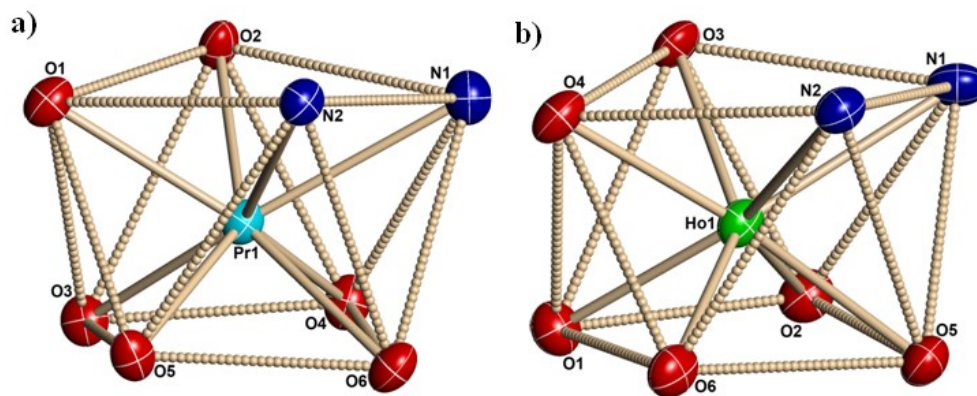**Fig. S1** FT-IR spectra of **1** (a) and **2** (b).

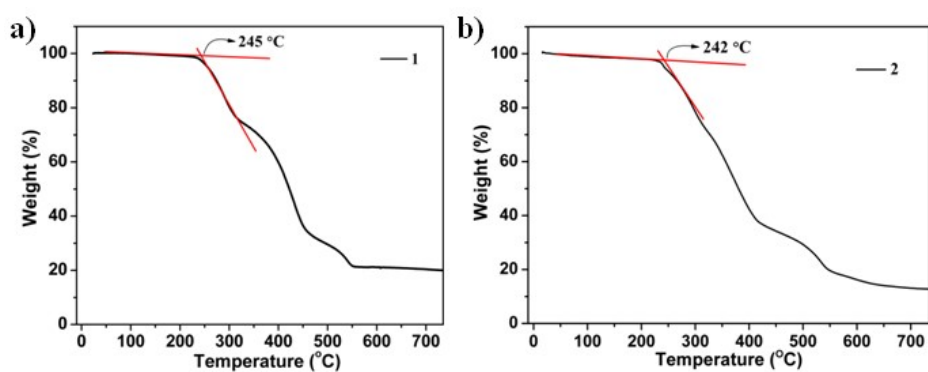**Fig. S2** Coordination geometries of Pr^III in **1** (a) and Ho^III in **2** (b).

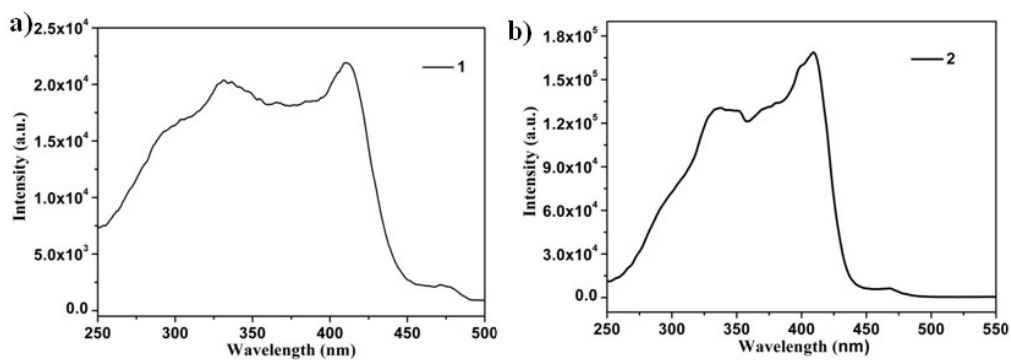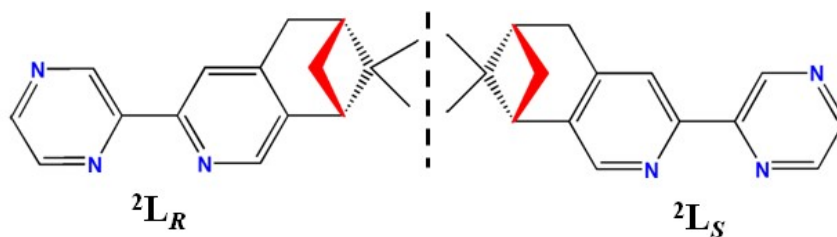**Fig. S3** Thermogravimetric analyses of **1** (a) and **2** (b).

Fig. S4 Excitation spectra of **1** (a) and **2** (b) obtained by monitoring their respective maximum emission wavelengths.

Scheme S1 Chemical structures of enantiopure N^N-donor ligands ²L_R and ²L_S.

Table S1 Crystallographic data and structure refinement parameters for **1** and **2**.

Complexes	**1**	**2**
Chemical formula	$C_{62}H_{51}N_2O_6Pr$	$C_{62}H_{51}N_2O_6Ho$
Formula weight	1060.95	1084.97
Crystal system	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$
a (Å)	9.5474(5)	9.5036(4)
b (Å)	20.9047(10)	20.7058(8)
c (Å)	12.6813(8)	12.7856(9)
α (deg)	90	90
β (deg)	92.922(5)	92.003(5)
γ (deg)	90	90
V (Å^3)	2527.7(2)	2514.4(2)
Z	2	2
D_c (g cm^{-3})	1.394	1.433
μ (mm^{-1})	1.019	1.629
F(000)	1088	1104
Reflections collected	9016	9303
Independent reflections	6656	6462
Data/restraints/parameters	6656/1/642	6462/1/642
GOF	0.894	1.024
$R_1[I >= 2\sigma(I)]^a$	0.0284	0.0288
w$R_2[I >= 2\sigma(I)]^b$	0.0312	0.0432
Flack parameter	0.001(9)	0.002(8)
CCDC	2351265	2351267

[a]$R_1 = \sum||Fo|-|Fc||/\sum|Fo|$. [b]w$R_2 = [\sum w(Fo^2 - Fc^2)^2/\sum w(Fo^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) and angles (°) for **1** and **2**.

Bond lengths for **1**

Pr(1)—O(1)	2.413(4)	Pr(1)—O(2)	2.430(5)	Pr(1)—O(3)	2.402(3)
Pr(1)—O(4)	2.416(2)	Pr(1)—O(5)	2.395(4)	Pr(1)—O(6)	2.418(5)
Pr(1)—N(1)	2.672(3)	Pr(1)—N(2)	2.659(3)		

Bond lengths for **2**

Ho(1)—O(1)	2.306(4)	Ho(1)—O(2)	2.317(3)	Ho(1)—O(3)	2.327(6)
Ho(1)—O(4)	2.322(5)	Ho(1)—O(5)	2.333(6)	Ho(1)—O(6)	2.296(5)
Ho(1)—N(1)	2.563(4)	Ho(1)—N(2)	2.539(4)		

Bond angles for **1**

O(3)-Pr(1)-O(2)	81.86(13)	O(3)-Pr(1)-O(5)	80.27(11)	O(6)-Pr(1)-O(5)	69.40(18)
O(1)-Pr(1)-O(3)	77.36(11)	O(6)-Pr(1)-N(1)	72.4(2)	O(3)-Pr(1)-N(2)	149.80(11)

Bond angles for **2**

O(3)-Ho(1)-O(2)	76.9(3)	O(3)-Ho(1)-O(5)	142.17(12)	O(6)-Ho(1)-O(5)	72.2(2)
O(1)-Ho(1)-O(3)	83.03(18)	O(6)-Ho(1)-N(1)	132.4(2)	O(3)-Ho(1)-N(2)	104.75(17)

Table S3 Continuous shape measures calculation for Pr1 in **1**.

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	29.146	22.002	17.063	10.401	**0.886**	1.808	15.043	27.024	2.519	1.932	4.464	11.007	22.568

Table S4 Continuous shape measures calculation for Ho1 in **2**.

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	28.890	22.740	16.662	10.020	**0.570**	1.720	15.558	27.743	2.289	1.772	4.414	10.751	23.319