Electronic Supplementary Information (ESI)

Multifunctional Zn(II)-Yb(III) complex enantiomers showing second-harmonic generation, near-infrared luminescence, singlemolecule magnet and proton conduction

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Complex <i>S</i> -1 (bond)	lengths (Å)	(angle)	angles (°)
Yb(1)-O(3)	2.227(2)	O(3)-Yb(1)-O(3)#1	132.47(11)
Yb(1)-O(3)#1	2.227(2)	O(3)-Yb(1)-O(2)	71.84(7)
Yb(1)-O(2)	2.265(2)	O(3)-Yb(1)-O(2)#1	154.02(7)
Yb(1)-O(2)#1	2.265(2)	O(1W)#1-Yb(1)-O(1)	134.07(8)
Yb(1)-O(1W)	2.306(2)	O(2W)-Zn(1)-O(3)	113.51(12)
Yb(1)-O(1W)#1	2.306(2)	O(2W)-Zn(1)-N(1)	117.15(13)
Yb(1)-O(1)#1	2.579(2)	O(3)-Zn(1)-N(1)	129.03(10)
Yb(1)-O(1)	2.579(2)	O(2W)-Zn(1)-N(2)	101.42(12)
Zn(1)-O(3)	2.010(2)	O(3)-Zn(1)-N(2)	91.29(9)
Zn(1)-N(1)	2.061(2)	N(1)-Zn(1)-N(2)	84.25(10)
Zn(1)-N(2)	2.139(3)		
Zn(1)-O(2)	2.152(2)		
Complex <i>R</i> -1 (bond)	lengths (Å)	(angle)	angles (°)
Complex <i>R</i> -1 (bond) Yb(1)-O(2)	lengths (Å) 2.268(5)	(angle) O(2)-Yb(1)-O(2)#1	angles (°) 86.59(12)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1	lengths (Å) 2.268(5) 2.268(5)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2)	angles (°) 86.59(12) 71.65(8)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1 Yb(1)-O(1W)	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6) 2.306(6)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2) O(2W)-Zn(1)-N(2)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14) 100.06(15)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1 Yb(1)-O(1W) Yb(1)-O(1)#1	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6) 2.306(6) 2.567(6)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2) O(2W)-Zn(1)-N(2) O(3)-Zn(1)-N(1)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14) 100.06(15) 128.89(11)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1 Yb(1)-O(1W) Yb(1)-O(1)#1 Yb(1)-O(1)#1	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6) 2.306(6) 2.567(6) 3.220(4)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2) O(2W)-Zn(1)-O(2) O(3)-Zn(1)-N(1) O(2W)-Zn(1)-N(1)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14) 100.06(15) 128.89(11) 117.25(16)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1 Yb(1)-O(1W) Yb(1)-O(1)#1 Yb(1)-C(10)#1 Zn(1)-O(2W)	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6) 2.306(6) 2.567(6) 3.220(4) 2.001(7)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2) O(2W)-Zn(1)-O(2) O(3)-Zn(1)-N(1) O(2W)-Zn(1)-N(1) N(1)-Zn(1)-O(2)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14) 100.06(15) 128.89(11) 117.25(16) 92.76(10)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1 Yb(1)-O(1W) Yb(1)-O(1)#1 Yb(1)-C(10)#1 Zn(1)-O(2W) Zn(1)-N(2)	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6) 2.306(6) 2.567(6) 3.220(4) 2.001(7) 2.159(6)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2) O(2W)-Zn(1)-O(2) O(3)-Zn(1)-N(1) O(2W)-Zn(1)-N(1) N(1)-Zn(1)-O(2) N(1)-Zn(1)-N(2)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14) 100.06(15) 128.89(11) 117.25(16) 92.76(10) 83.82(12)
Complex <i>R</i>-1 (bond) Yb(1)-O(2) Yb(1)-O(2)#1 Yb(1)-O(3) Yb(1)-O(3)#1 Yb(1)-O(1W)#1 Yb(1)-O(1W) Yb(1)-O(1)#1 Yb(1)-C(10)#1 Zn(1)-O(2W) Zn(1)-N(2) Zn(1)-N(1)	lengths (Å) 2.268(5) 2.268(5) 2.228(5) 2.228(5) 2.306(6) 2.306(6) 2.567(6) 3.220(4) 2.001(7) 2.159(6) 2.060 (3)	(angle) O(2)-Yb(1)-O(2)#1 O(3)-Yb(1)-O(2) O(3)-Yb(1)-O(2)#1 O(2)-Yb(1)-O(1W)#1 O(2W)-Zn(1)-O(2) O(2W)-Zn(1)-O(2) O(3)-Zn(1)-N(1) O(2W)-Zn(1)-N(1) N(1)-Zn(1)-O(2) N(1)-Zn(1)-N(2)	angles (°) 86.59(12) 71.65(8) 153.76(8) 85.35(10) 95.51(14) 100.06(15) 128.89(11) 117.25(16) 92.76(10) 83.82(12)

 Table S1. Selected bond lengths (Å) and angles (°) for S-1 and R-1

^{*a*}Symmetry Codes for **S-1**: #1 x, -y+1, -z+1; for **R-1**: #1 x, -y, -z, #2 -x+1, y, -z+1/2

label	shape	symmetry	$Distortion(\tau)$
OP-8	Octagon	D_{8h}	83.902
HPY-8	Heptagonal pyramid	C_{7v}	78.842
HBPY-8	Hexagonal bipyramid	D _{6h}	80.452
CU-8	Pentagonal prism	O_h	79.304
SAPR-8	Square antiprism	D_{4d}	77.131
TDD-8	Square antiprism	D_{2d}	77.136
JGBF-8	Johnson gyrobifastigium J26	D_{2d}	79.909
JETBPY-8	Johnson elongated triangular bipyramid J14	D_{3h}	82.886
JBTPR-8	Biaugmented trigonal prism J50	C_{2v}	74.301
BTPR-8	Biaugmented trigonal prism	C_{2v}	74.979
JSD-8	Snub diphenoid J84	D_{2d}	77.273
TT-8	Triakis tetrahedron	T_d	79.308
ETBPY-8	Elongated trigonal bipyramid	D_{3h}	82.271

Table S2 Summary of SHAPE analysis for *S*-1.

 Table S3. Hydrogen-bonding geometry for S-1.

D−Н…А	D−H···A (Å)	∠(DHA) (°)
N2-H2…O6	3.216(6)	163
O1W-H1WA…O8	2.933(5)	152
N1–H1…O9	3.207(5)	163
N2–H2…O7	3.362(7)	145
O2W-H2WB…O6	3.164(7)	154
O2W-H2WA…O5W	3.148(8)	148
O2W-H2WB…O4W	3.275(8)	138
O3W-H3W···O2W	2.744(4)	153
O4W-H4WB…O5W	2.760(3)	138
O5W–H5WA…O4W	2.760(3)	100
O5W−H5WB…O7	3.158(1)	75



Fig. S1. The 3-D supramolecular network of *S*-1 formed by H-bonds interactions (green dashed lines) between imine (N1) of *SS*-L²- ligandand perchlorate anions (N1 \cdots O9 = 3.210 (5) Å), and the lattice water molecules (O2W \cdots O3W = 3.214(9) Å). The other H-bonds are omitted for clarity.



Fig. S2. The TGA plot of *S*-1.



Fig. S3. Solid-state excitation spectra for *S*-1 at room temperature.



Fig. S4. Temperature dependence of magnetic susceptibility for S-1.



Fig. S5. The *M* vs. *H* plot of *S*-1.



Fig. S6. The solid state of UV spectra for *S*-1.

