A Pair of Homochiral Trinuclear Zn (II) Clusters Exhibiting Unusual Ferroelectric Behavior at High-Temperature

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Electronic Supplementary Information

Content

Table S1 Crystallographic data and structure refinement for **R-1** and **S-1**

Name	**S-1**	**R-1**
Empirical formula	C_{40} H_{44} N_2 O_{12} Zn_3	C_{40} H_{44} N_2 O_{12} Zn_3
Formula weight	940.88	940.88
Temperature/K	293.15	173
Wavelength/Å	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
space group	$P2_1$	$P2_1$
a/Å	10.5958(17)	10.4740(5)
b/Å	17.944(2)	17.8233(9)
c/Å	11.8027(19)	11.7087(5)
α/°	90	90
β/°	107.323(6)	107.0091(13)
γ/°	90	90
Volume/Å^3	2142.2(6)	2090.18(17)
Z	2	2
ρ_{calc}mg/cm^3	1.459	1.495
Absorption coefficient/mm^{-1}	1.727	1.770
F(000)	968	968
Crystal size/ mm^3	0.03 x 0.02 x 0.01	0.03 x 0.02 x 0.01
Theta range for data collection/°	2.90 to 25.20	2.92 to 28.32
Index ranges	-12<=h<=12 -21<=k<=21 -14<=l<=14	-13<=h<=13 -23<=k<=23 -15<=l<=15
Reflections collected	31417	48441
Independent reflections	7681 [R(int) = 0.0259]	10317 [R(int) = 0.0208]
Completeness to theta = 25.20	99.8%	99.6%
Max. and min. transmission	0.7457 and 0.6050	0.7457 and 0.6158
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints / parameters	7681 / 1 / 522	10317 / 1 / 522
Goodness-of-fit on F^2	1.069	1.059
Final R indices [I>2sigma(I)]	R_1 = 0.0658, wR_2 = 0.1942	R_1 = 0.0600, wR_2 = 0.1833
R indices (all data)	R_1 = 0.0692, wR_2 = 0.1991	R_1 = 0.0621, wR_2 = 0.1860
Absolute structure parameter	0.08(2)	0.068(15)

Largest diff. peak/hole / e Å^{-3}	0.583/-2.686	0.890/-3.823

Table S2. Main bond lengths (Å) for **S-1** and **R-1**

Bond lengths (Å)			
S-1		**R-1**	
Zn(1)-N(1)	2.021(6)	Zn(1)-N(1)	2.006(4)
Zn(1)-O(2)	1.941(4)	Zn(1)-O(2)	1.934(3)
Zn(1)-O(3)	1.963(5)	Zn(1)-O(4)	1.961(4)
Zn(1)-O(4)	1.933(5)	Zn(1)-O(5)	1.939(4)
Zn(2)-O(2)	2.420(5)	Zn(2)-O(2)	2.419(4)
Zn(2)-O(5)	2.361(5)	Zn(2)-O(3)	2.361(4)
Zn(2)-O(6)	2.361(6)	Zn(2)-O(6)	2.361(4)
Zn(2)-O(7)	2.428(6)	Zn(2)-O(7)	2.426(4)
Zn(2)-O(10)	2.353(6)	Zn(2)-O(10)	2.357(4)
Zn(2)-O(11)	2.428(5)	Zn(2)-O(11)	2.427(4)
Zn(3)-O(8)	1.926(6)	Zn(3)-O(8)	1.939(4)
Zn(3)-O(9)	1.944(6)	Zn(3)-O(9)	1.950(4)
Zn(3)-O(11)	1.963(5)	Zn(3)-O(11)	1.953(4)
Zn(3)-N(2)	2.027(6)	Zn(3)-N(2)	2.020(5)

Table S3. Main bond angles (°) for **S-1** and **R-1**

Bond angles (°)			
S-1		**R-1**	
O(2)-Zn(1)-N(1)	96.7(2)	O(2)-Zn(1)-N(1)	96.77(16)
O(2)-Zn(1)-O(3)	111.0(2)	O(2)-Zn(1)-O(4)	110.60(16)
O(4)-Zn(1)-N(1)	115.0(2)	O(2)-Zn(1)-O(5)	112.72(17)
O(4)-Zn(1)-O(2)	112.3(2)	O(4)-Zn(1)-N(1)	110.02(17)
O(4)-Zn(1)-O(3)	110.7(2)	O(5)-Zn(1)-N(1)	115.49(17)
O(3)-Zn(1)-N(1)	110.5(2)	O(5)-Zn(1)-O(4)	110.55(18)
O(2)-Zn(2)-O(7)	153.35(18)	O(2)-Zn(2)-O(11)	130.55(13)

O(2)-Zn(2)-O(11)	130.16(17)	O(2)-Zn(2)-O(7)	153.16(13)
O(5)-Zn(2)-O(2)	75.98(19)	O(7)-Zn(2)-O(11)	74.60(13)
O(5)-Zn(2)-O(7)	81.7(2)	O(3)-Zn(2)-O(11)	110.48(14)
O(5)-Zn(2)-O(11)	151.87(19)	O(3)-Zn(2)-O(2)	78.93(13)
O(7)-Zn(2)-O(11)	75.00(18)	O(3)-Zn(2)-O(7)	83.13(14)
O(10)-Zn(2)-O(2)	108.4(2)	O(3)-Zn(2)-O(6)	82.01(16)
O(10)-Zn(2)-O(5)	82.4(2)	O(6)-Zn(2)-O(11)	150.73(14)
O(10)-Zn(2)-O(7)	82.5(2)	O(6)-Zn(2)-O(2)	76.81(14)
O(10)-Zn(2)-O(11)	79.20(19)	O(6)-Zn(2)-O(7)	81.08(14)
O(10)-Zn(2)-O(6)	160.2(2)	O(10)-Zn(2)-O(11)	79.49(13)
O(6)-Zn(2)-O(2)	79.37(17)	O(10)-Zn(2)-O(2)	108.64(14)
O(6)-Zn(2)-O(5)	82.0(2)	O(10)-Zn(2)-O(7)	82.61(15)
O(6)-Zn(2)-O(7)	83.3(2)	O(10)-Zn(2)-O(3)	159.63(15)
O(6)-Zn(2)-O(11)	110.24(19)	O(10)-Zn(2)-O(6)	81.48(16)
O(8)-Zn(3)-O(11)	112.2(2)	O(11)-Zn(3)-N(2)	95.05(17)
O(8)-Zn(3)-O(9)	110.0(3)	O(9)-Zn(3)-N(2)	107.7(2)
O(8)-Zn(3)-N(2)	115.9(3)	O(9)-Zn(3)-O(11)	115.55(17)
O(11)-Zn(3)-N(2)	95.2(2)	O(8)-Zn(3)-N(2)	115.63(18)
O(9)-Zn(3)-O(11)	115.3(2)	O(8)-Zn(3)-O(11)	112.30(17)
O(9)-Zn(3)-N(2)	107.6(3)	O(8)-Zn(3)-O(9)	110.0(2)

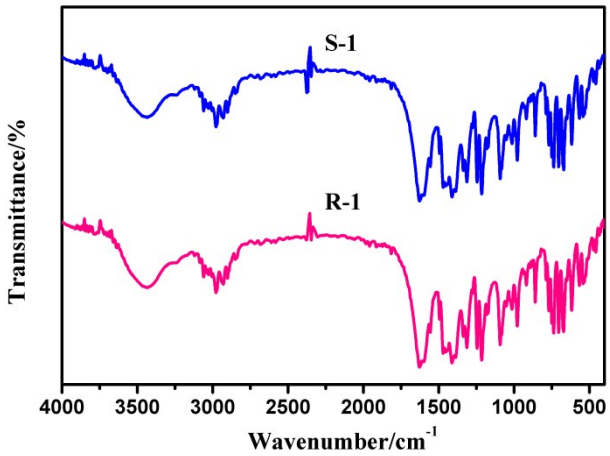

Fig.S1 IR spectra for **S-1** and **R-1** at RT in KBr pellets

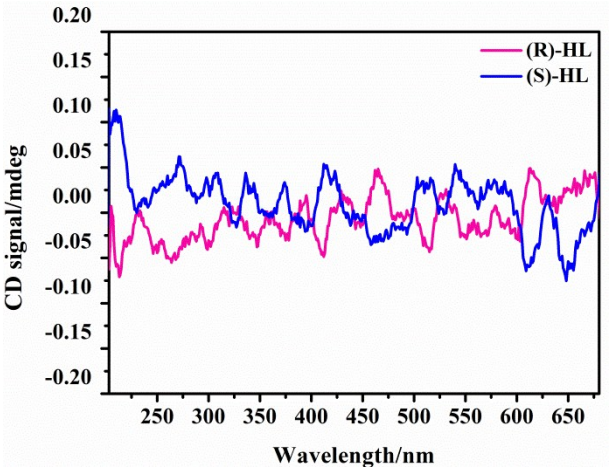

Fig. S2 CD spectra for (R)-HL and (S)-HL solution (1×10^{-2} mmol/mL, CH_3OH)

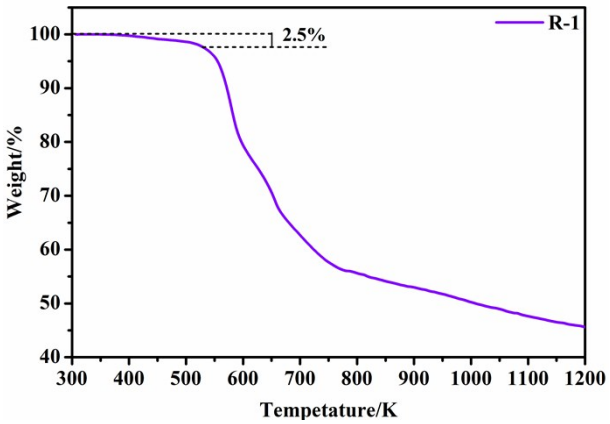

Fig.S3 Thermogravimetric curves for **R-1**

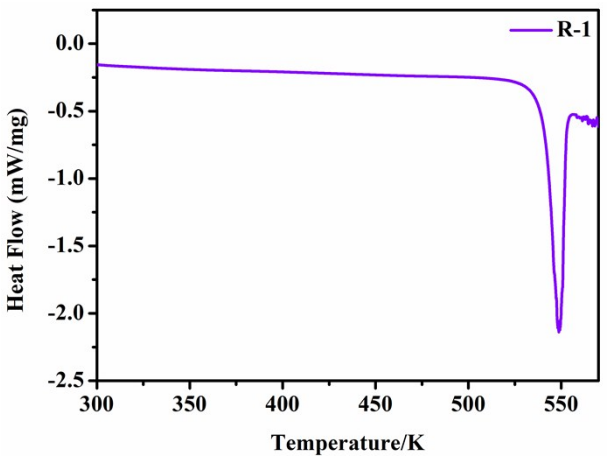

Fig.S4 DSC curves for **R-1**

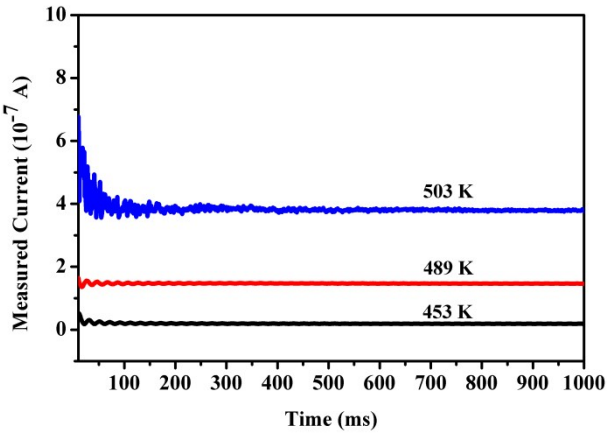

Fig.S5 The leakage current for **R-1** at 1200 V under different temperature

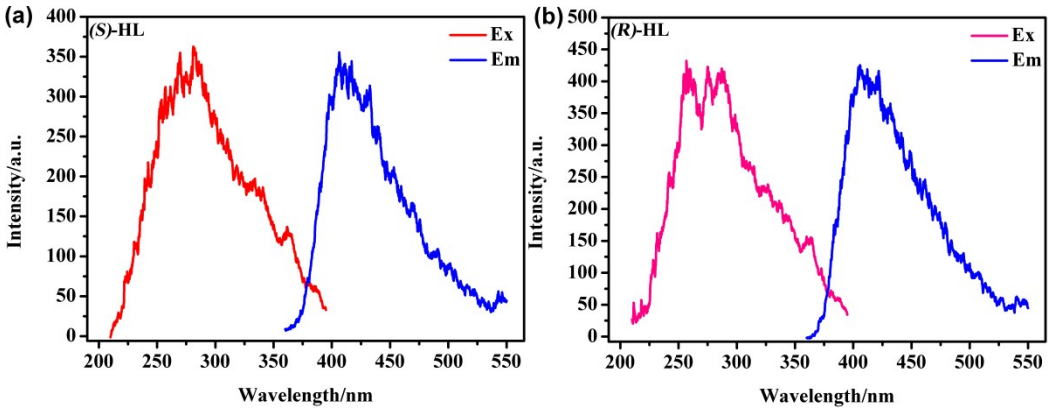

Fig.S6 The fluorescence spectra of (R)-**HL** (a) and (R)-**HL** (b) at room temperature (1×10^{-5} M)

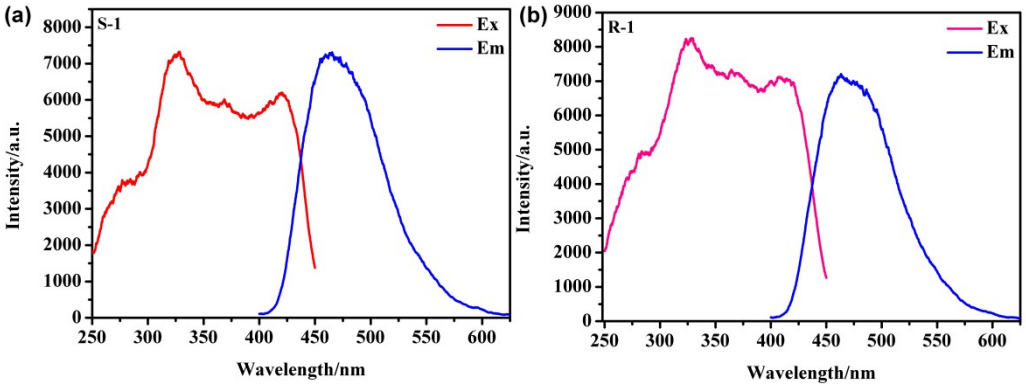

Fig.S7 The solid-state fluorescence spectra of **S-1** (a) and **R-1** (b) at room temperature

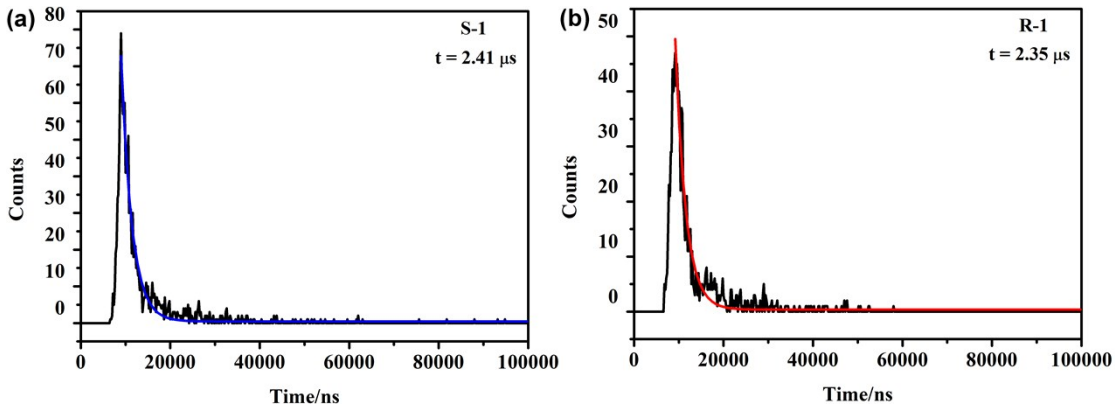

Fig.S8 The fluorescent lifetime for **S-1** and **R-1**