Supporting information

Metal-Organic Ferroelectric Complexes: Enantiomer Directional Induction Achieved Above-Room-Temperature Homochiral Molecular Ferroelectrics

Jia-Zhen Ge, # Yu-Ling Liu, # Zhong-Xia Wang* and Ren-Gen Xiong*

[‡]These authors contributed equally to this work.



Fig. S1 Pattern of powder X-ray diffraction of *R*-configuration at 298 K, verifying the purity of the bulk phase.



Fig. S2 Pattern of powder X-ray diffraction of *S*-configuration at 298 K, verifying the purity of the bulk phase.



Fig. S3 DFT calculated VCD and IR spectra for *R*- and *S*-configuration.



Fig. S4 Temperature-dependent dielectric real part ε' under 1000 kHz in a heating and cooling cycle with the same heating/cooling rate of 15 K min⁻¹ in terms of polycrystalline samples for *R*- and *S*-configuration.



Fig. S5 Comparison of ferroelectric P-E loop of S-configuration and racemate at 318 K.



Fig. S6 Domain properties of the thin film of *R*-configuration. Vertical phase (a) and amplitude images (b) and topographic images (c) for the thin film. (d) Phase and amplitude signals as functions of the tip voltage for a selected point, showing local PFM hysteresis loops.

Compound	R-configuration	R -configuration	S-configuration	S-configuration
Formula weight	643.01	643.01	643.01	643.01
Temperature	293 K	373 K	298 K	373 K
Crystal system	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	<i>P</i> 1	<i>C</i> 2	<i>P</i> 1	C2
a/Å	10.960(7)	17.62(4)	10.9605(9)	17.5768(14)
b/Å	11.018(7)	13.23(3)	10.9825(9)	13.1751(7)
c/Å	12.933(9)	13.36(3)	12.9788(9)	13.3367(10)
α/deg	101.979(4)	90	102.213(5)	90
β/deg	113.103(7)	123.10(5)	113.419(5)	123.110(7)
γ/deg	106.145(5)	90	106.1900	90
Volume/Å ³	1288.2(15)	2609(10)	1281.33	2587.0(4)
Ζ	2	4	2	4
Density/g cm ⁻³	1.658	1.635	1.667	1.648
$R_1 \left[I \ge 2\sigma(I) \right]$	0.0454	0.0614	0.0590	0.0421
$wR_2 [I \ge 2\sigma(I)]$	0.0921	0.1469	0.1528	0.0932
GOF	0.975	1.001	1.018	1.000

 Table S1 Crystal data and structure refinements for *R*- and *S*-configuration.