

Supporting Information

Chiral Star-Shaped [Co₃Ln] Clusters Based on Enantiomeric Schiff Bases: Synthesis, Crystal Structures, and Magnetic Properties

Liudi Ji,^{1,2} Juntao Wang,^{1,2} Zeyu Li,^{1,2} Xiaoming Zhu,^{*1,2} Peng Hu^{*1,2}

¹School of Nuclear Technology and Chemistry & Biology, Hubei University of Science and Technology, Xianning 437100, China

²Hubei Key Laboratory of Radiation Chemistry and Functional Materials, Hubei University of Science and Technology, Xianning 437100, China

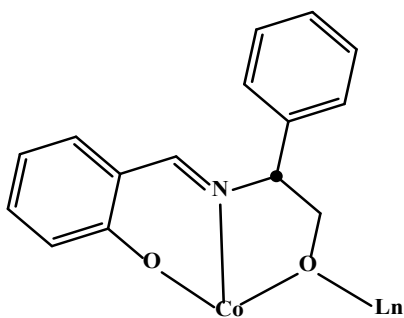


Figure S1. Coordination modes of Ligands *R-/S*-H₂L in this work.

Table S1 Crystal data and structure refinements for **1R**, **1S**, **2R** and **2S**.

Complexes	1R	1S	2R	2S
Formula	C ₉₀ H ₇₈ Co ₃ DyN ₆ O ₁₂	C ₉₀ H ₇₈ Co ₃ DyN ₆ O ₁₂	C ₉₀ H ₇₈ Co ₃ GdN ₆ O ₁₂	C ₉₀ H ₇₈ Co ₃ GdN ₆ O ₁₂
Formula weight	1774.88	1774.88	1769.63	1769.63
Temp (K)	100.00(10)	100.00(10)	100.01(10)	100.00(10)
Crystal system	cubic	cubic	cubic	cubic
Space group	<i>P</i> 2 ₁ 3	<i>P</i> 2 ₁ 3	<i>P</i> 2 ₁ 3	<i>P</i> 2 ₁ 3
<i>a</i> (Å)	21.3246(2)	21.217(3)	21.2867(2)	21.3623(3)
<i>b</i> (Å)	21.3246(2)	21.217(3)	21.2867(2)	21.3623(3)
<i>c</i> (Å)	21.3246(2)	21.217(3)	21.2867(2)	21.3623(3)
<i>α</i> (deg)	90	90	90	90
<i>β</i> (deg)	90	90	90	90
<i>γ</i> (deg)	90	90	90	90
<i>V</i> (Å ³)	9697.1(3)	9551 (3)	9645.5(3)	9645.5(3)
<i>Z</i>	4	4	4	4
<i>D_c</i> (g cm ⁻³)	1.214	1.234	1.219	1.206
<i>M</i> (mm ⁻¹)	8.445	8.574	8.793	8.700
<i>F</i> (000)	3600.0	3612.0	3604.0	3604.0
no. of rflns collected	6587	6487	6537	6613
no. of unique rflns	3565	3513	3539	3579
no. params	331	337	337	337
GOF	1.051	0.993	1.115	0.993
<i>R</i> ₁ , ^{<i>a</i>} <i>wR</i> ₂ ^{<i>b</i>} [<i>I</i> > 2σ(<i>I</i>)]	0.0986, 0.2538	0.0896, 0.2403	0.1066, 0.2717	0.0896, 0.2403
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.1145, 0.2660	0.1084, 0.2249	0.1198, 0.2824	0.1084, 0.2249
Flack parameter	0.011(7)	0.008(6)	0.013(7)	0.008(6)
CCDC	2348361	2348363	2348362	2348364

^{*a*}*R*₁ = $\sum||F_o| - |F_c||/\sum|F_o|$. ^{*b*}*wR*₂ = $[\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)_2]^{1/2}$.

Table S2 Selected Bond Distances (Å) and Angles (°) for **1R**, **1S**, **2R** and **2S**.

Compound	1R	1S	1R	1S
Ln-O1	2.179(6)	2.163(7)	2.208(6)	2.167(7)
Ln-O2	2.194(6)	2.208(6)	2.248(6)	2.203(7)
Ln-O3	2.179(6)	2.163(7)	2.208(6)	2.167(7)
Ln-O4	2.194(6)	2.208(6)	2.248(6)	2.203(7)
Ln-O5	2.179(6)	2.163(7)	2.208(6)	2.167(7)
Ln-O6	2.194(6)	2.208(6)	2.248(6)	2.203(7)
O1- Ln-O2	72.1(2)	71.9(2)	71.3(2)	72.1(3)
O1- Ln-O3	91.2(2)	91.8(2)	91.6(2)	91.2(2)
O1- Ln-O4	149.4(3)	149.7(2)	149.4(3)	149.8(3)

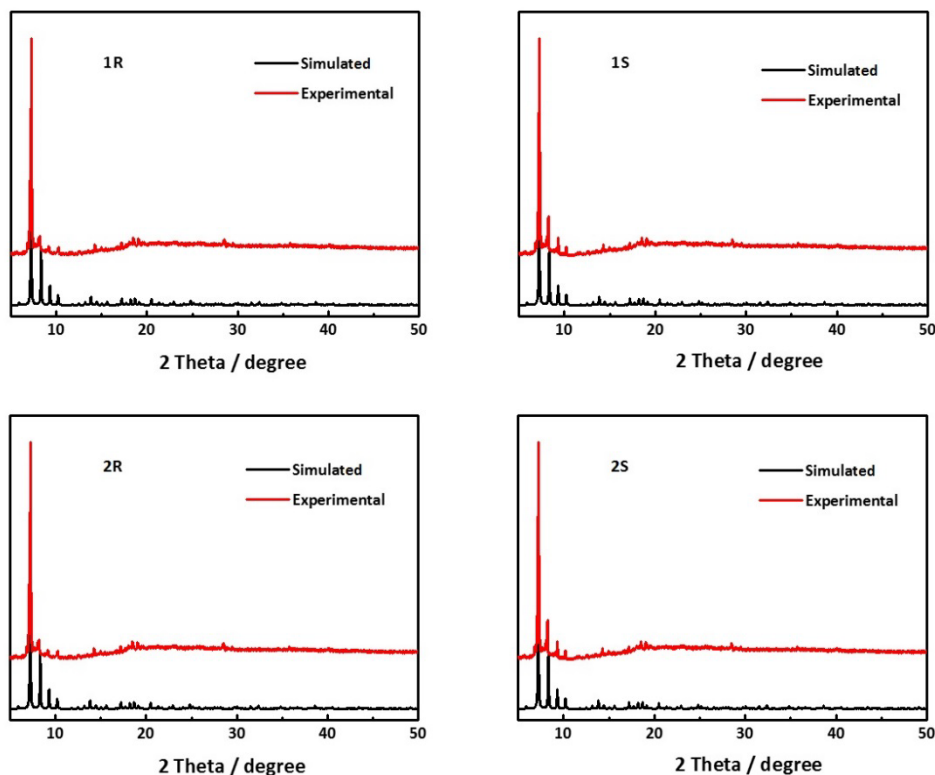


Figure S2. The simulated X-ray powder diffraction patterns (black) and the experimental ones (red) of compounds **1R**, **1S**, **2R** and **2S**. Powder X-ray diffraction (PXRD) of the crystalline samples of complexes **1R**, **1S**, **2R** and **2S** were carried out, and the results are shown in Figure S2. The experimental PXRD patterns are primarily consistent with the the corresponding simulated ones,

highlighting the phase purity of the four complexes. Minor inconsistencies in the intensity and shape of the peaks were observed between the experimental and simulation data due to the different orientations of the crystal samples.

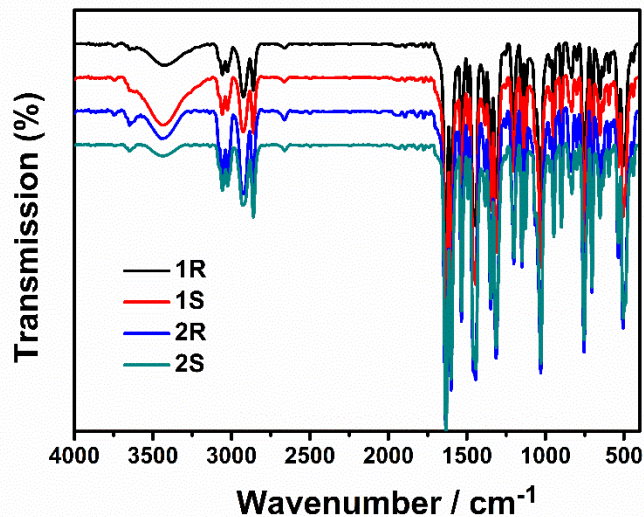


Figure S3. FT-IR spectra of **1R** (black), **1S** (red), **2R** (blue) and **2S** (green).

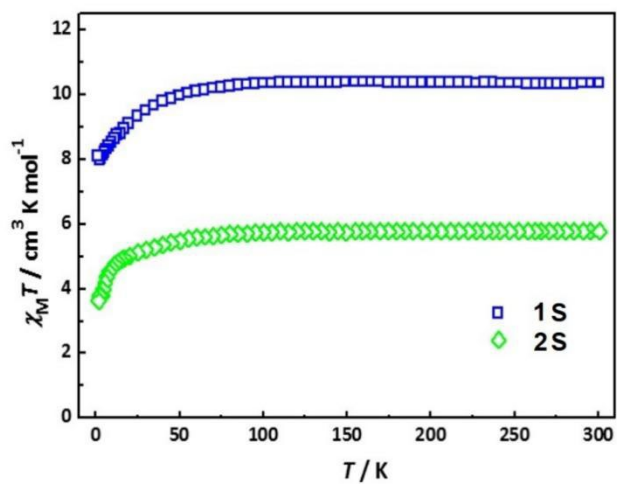


Figure S4. Plots of the temperature dependence of $\chi_M T$ vs. T for **1S** and **2S**.

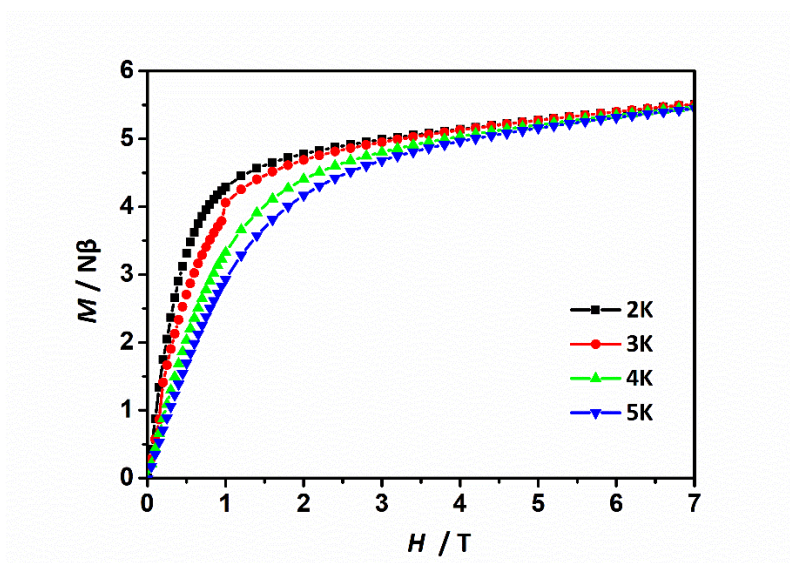


Figure S5. Magnetization curve for compound **1S** at different temperatures (2 K, 3 K, 4 K and 5 K).

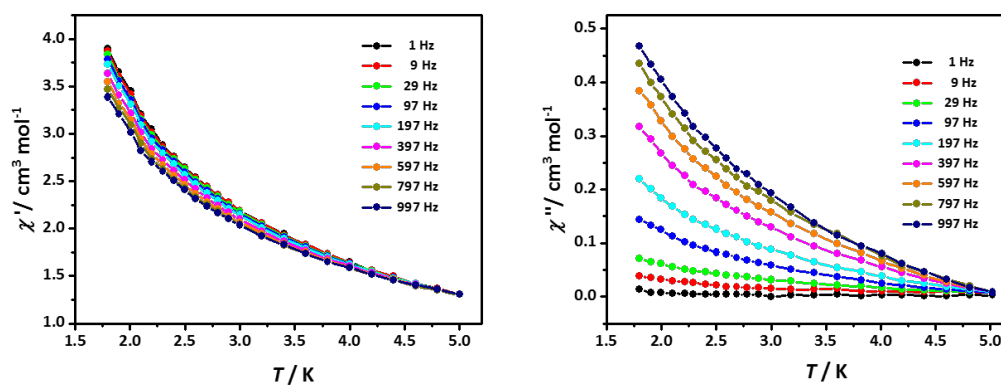


Figure S6. Temperature dependence of the in-phase (χ') (left) and out-of-phase (χ'') (right) ac susceptibility data for **1R** under a zero-dc field.

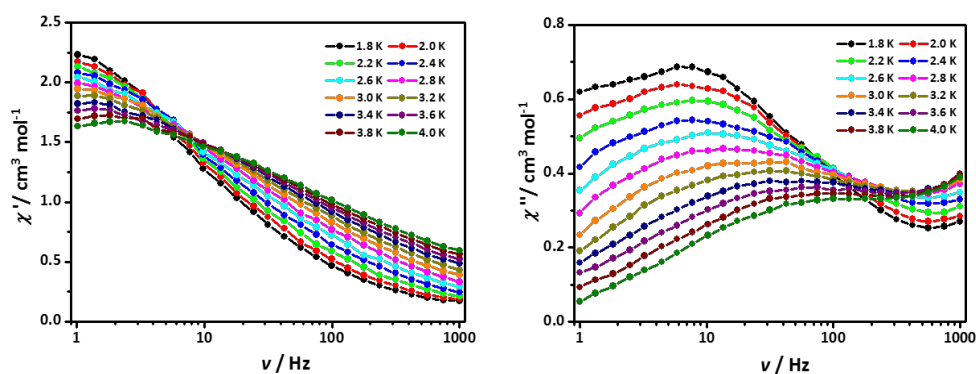


Figure S7. Frequency dependence of the in-phase (χ') (left) and out-of-phase (χ'') (right) ac susceptibility data for **1R** under a 2000 Oe applied dc field.

Table S3. The parameters obtained by fitting Cole-Cole plot under the optimal dc field for **1R**.

T (K)	χ_S	χ_T	τ	α
1.8	0.68	1.76	0.0172	0.26
2.0	0.63	1.68	0.0133	0.25
2.2	0.58	1.52	0.0099	0.23
2.4	0.52	1.35	0.0086	0.22
2.6	0.47	1.21	0.0072	0.22
2.8	0.42	1.13	0.0059	0.23
3.0	0.38	1.06	0.0050	0.21
3.2	0.36	1.02	0.0043	0.20
3.4	0.35	0.96	0.0037	0.19
3.6	0.34	0.90	0.0031	0.20
3.8	0.32	0.85	0.0025	0.19
4.0	0.31	0.82	0.0021	0.18

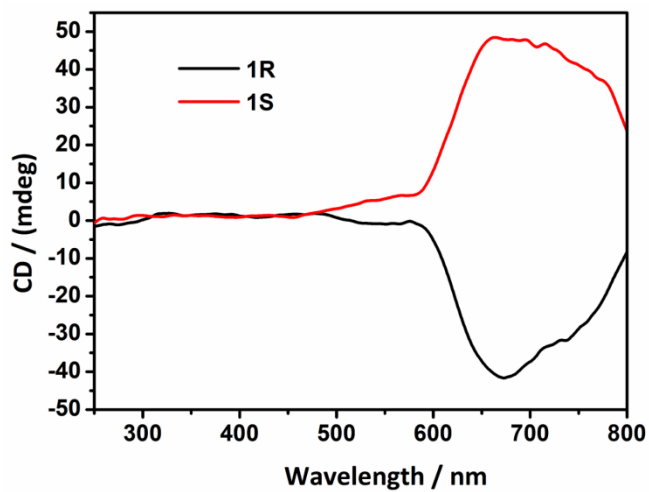


Figure S8. The solid-state CD spectra of **1R** and **1S** in KBr pellet at 298 K.