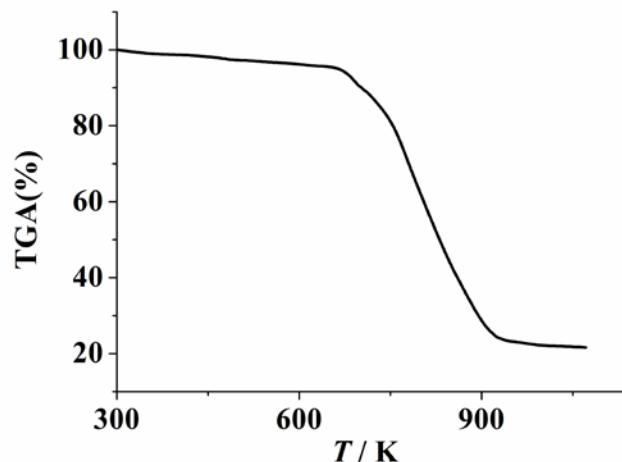


# Tuning the Spin States of Two Apical Iron(II) Ions in a Pentanuclear Iron(II) Cluster Helicate Through the Choice of Anions

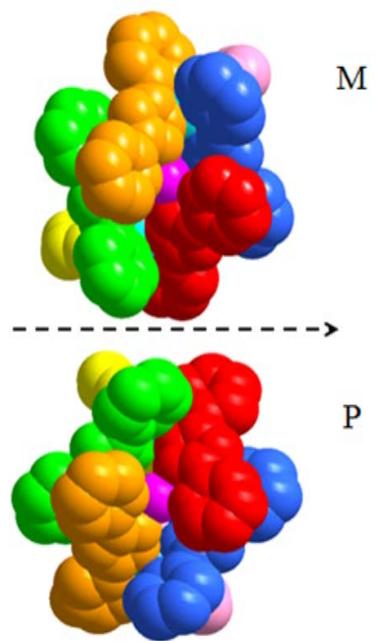
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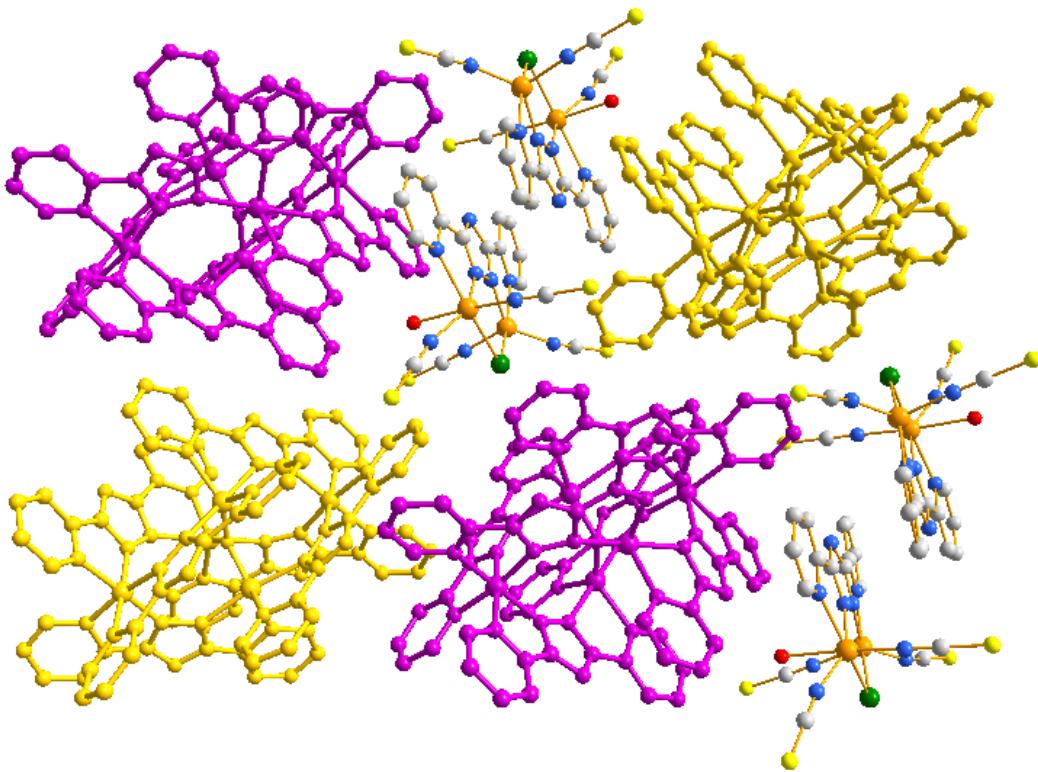
\* Corresponding author, E-mail addresses: [yzheng158@mail.zjxu.edu.cn](mailto:yzheng158@mail.zjxu.edu.cn)



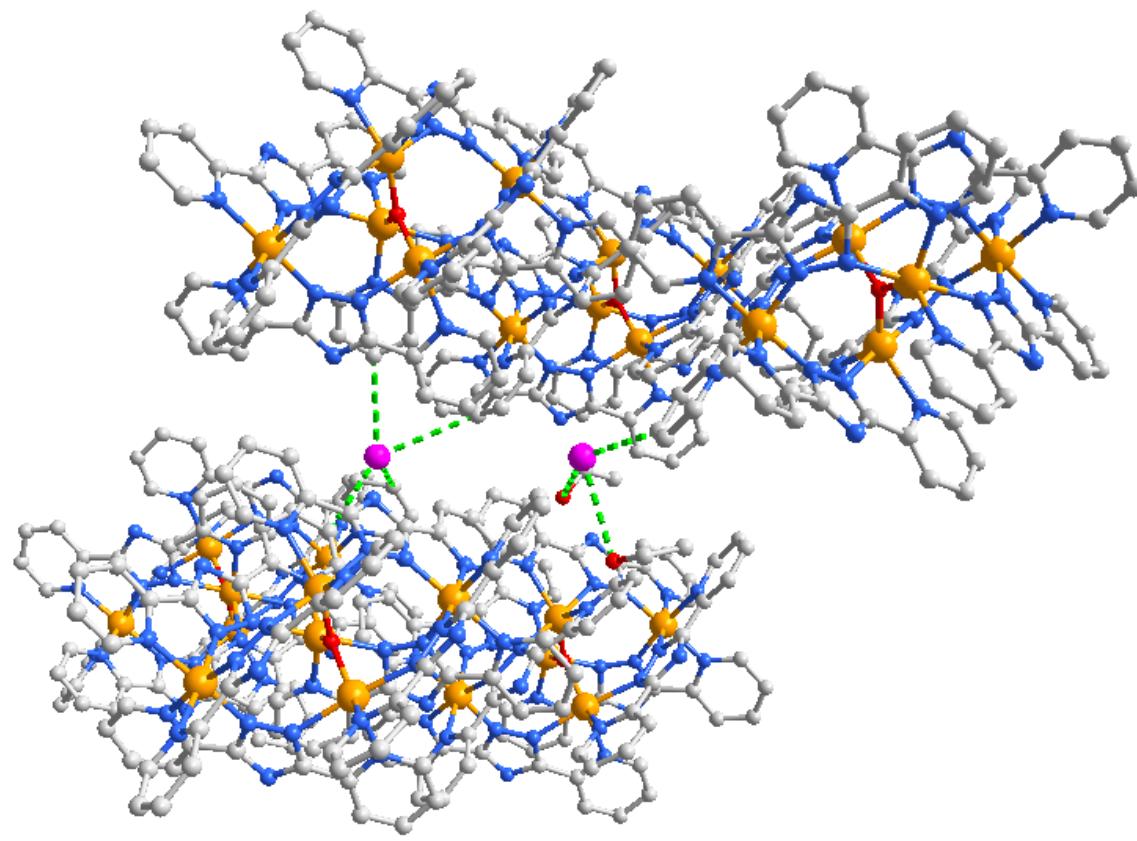
**Figure S1.** Thermogravimetric analysis of **1** under N<sub>2</sub> atmosphere (10 K min<sup>-1</sup>).



**Figure S2.** Space-filling representation of the two enantiomers present in **1**. H atoms are omitted for clarity.



**Figure S3.** Packing diagram of **1** showing heterochiral layers.  $\Delta, \Delta$ -configuration (right-handed, P) is shown in purple strands,  $\Lambda, \Lambda$ -configuration (left-handed, M) in yellow strands.



**Figure S4.** Structural illustrations of 3:the hydrogen bond interactions.

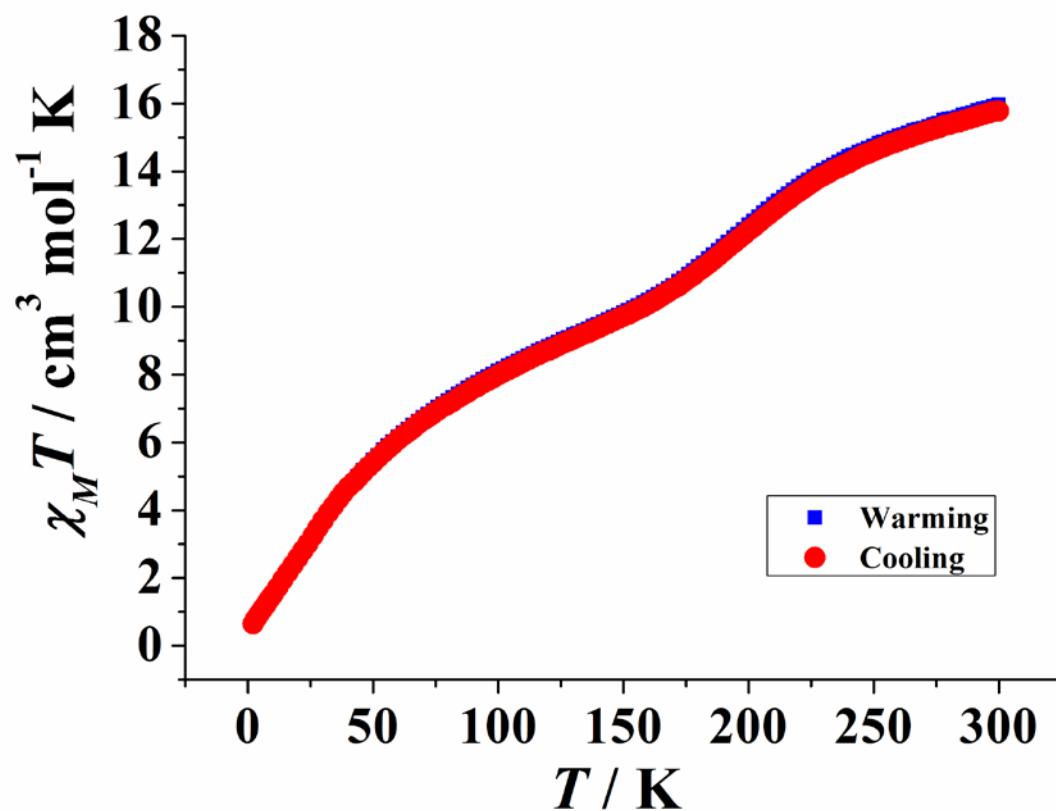
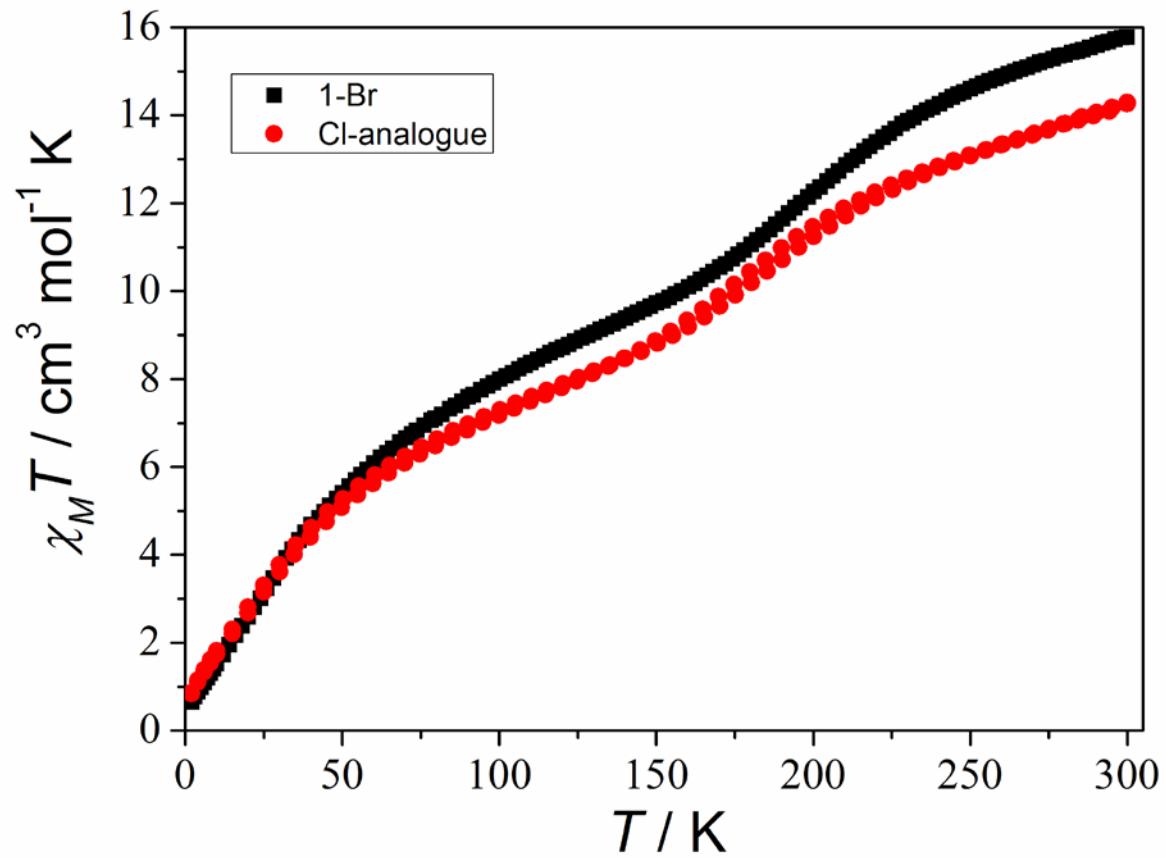


Figure S5. Plots of  $\chi_M T$  vs  $T$  for 1.



**Figure S6.** Plots of  $\chi_M T$  vs  $T$  for **1** and Cl-analogue.

**Table S1. Geometrical Parameters of Hydrogen Bond in Compound 1**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(10)	0.85	1.952	2.791	169.41
C(71)-H(71)...S(1)	0.950	2.978	3.909	166.88
O(2)-H(2)...S(1)	0.850	2.537	3.379	170.94
C(40)-H(40)...S(3)	0.952	2.788	3.385	157.90
C(23)-H(23)...S(2)	0.950	2.716	3.574	150.52
C(47)-H(47)...S(2)	0.949	2.861	3.810	177.48
C(49)-H(49)...S(1)	0.950	2.877	3.686	143.66
C(35)-H(35)...S(4)	0.950	2.968	3.840	153.14

Symmetry codes     $\frac{-x}{2}, \frac{y}{2}, \frac{z+1}{2}$      $\frac{-b}{2}, x, \frac{y}{2}$      $\frac{-1}{2}, c, x$      $\frac{-x+1}{2}, \frac{y+1}{2}, -z$      $\frac{-e}{2}, \frac{y}{2}, \frac{z}{2}$      $\frac{-f}{2}, x, y, \frac{-x+1}{2}, \frac{y+1}{2}$      $, z; h, x+1, y, z$ .

**Table S2. Geometrical Parameters of Hydrogen Bond in Compound 2**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(12)-H(12)...N(14)	0.95	2.59	3.1095	115
C(18)-H(18)...N(1)	0.95	3.00	3.9225	163
C(24)-H(24)...N(5)	0.95	2.61	3.1375	115
C(31)-H(31)...N(10)	0.95	2.58	3.1084	115
C(31)-H(31)...N(16)	0.95	2.58	3.3258	136

**Table S3. Geometrical Parameters of Hydrogen Bond in Compound 3**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17)...I(6a)	0.95	2.75	3.4796	134
C(18)-H(18)...I(2a)	0.95	2.82	3.6594	148

C(23)-H(23)...I(4 <i>b</i> )	0.95	2.74	3.5319	141
C(66)-H(66)...I(5)	0.95	2.77	3.5585	141
C(71)-H(71)...I(1 <i>c</i> )	0.95	2.74	3.6072	152

Symmetry codes: a) x, y-1, z; b) -x, -y+1, z; c) 1-x, y-1/2, -z+1/2