

Supporting Information for

A Ladder Type Iron(II) Coordination Polymer with Enhanced Spin-Crossover Behavior

Zheng Yan,^{a,b,*} Long-Feng Zhu,^b Lian-Wen Zhu,^b Yan Meng,^c Md. Najbul Hoque,^a Jun-Liang Liu,^a Yan-Cong Chen,^a Zhao-Ping Ni,^{a,*} Ming-Liang Tong^{a,*}

^a Key Laboratory of Bioinorganic and Synthetic Chemistry of Ministry of Education, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, P. R. China.

^b College of Biological, Chemical Sciences and Engineering, Jiaxing University, Jiaxing 314001, P. R. China

^c Anhui Key Laboratory of Functional Coordination Compounds, Anqing Normal University, Anqing 246011, P. R. China.

e-mail: yzheng158@163.com, nizhp@mail.sysu.edu.cn, tongml@mail.sysu.edu.cn

Contents of the Supporting Information

Scheme S1. The molecular structures of the ligands.

Figure S1. The PXRD spectrum of **2**.

Figure S2. Structural illustrations of **2** along the *c* axis highlighting the interchains C-H...C interactions and Au...Au interactions.

Figure S3. Photographs of single crystal of **2**.

Figure S4. Excess heat capacity associated with the SCO transition for **1·H₂O** upon warming.

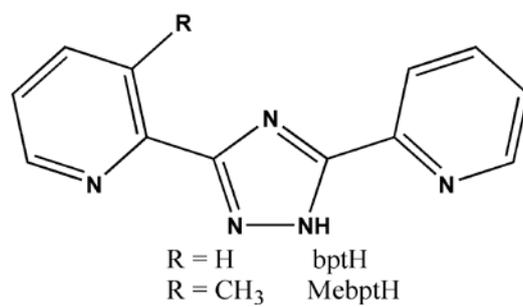
Figure S5. Crystal packing of **2** in the *ab* plane. The different Fe...Fe projection distances are given for LS **2**.

Figure S6. Crystal packing of **1·H₂O** in the *ac* plane. The different Fe...Fe projection distances are given for LS **1·H₂O**.

Figure S7. Structural illustrations of **2** highlighting the interchains offset face-to-face $\pi\cdots\pi$ interactions.

Figure S8. Structural illustrations of **1·H₂O** highlighting the interchains offset face-to-face $\pi\cdots\pi$ interactions.

Table S1. Fe...Fe projection distances observed in the three different crystallographic axes of the solid state structure of **2** and **1·H₂O**, and their variation upon LS \leftrightarrow HS transition.



Scheme S1. The molecular structures of the ligands.

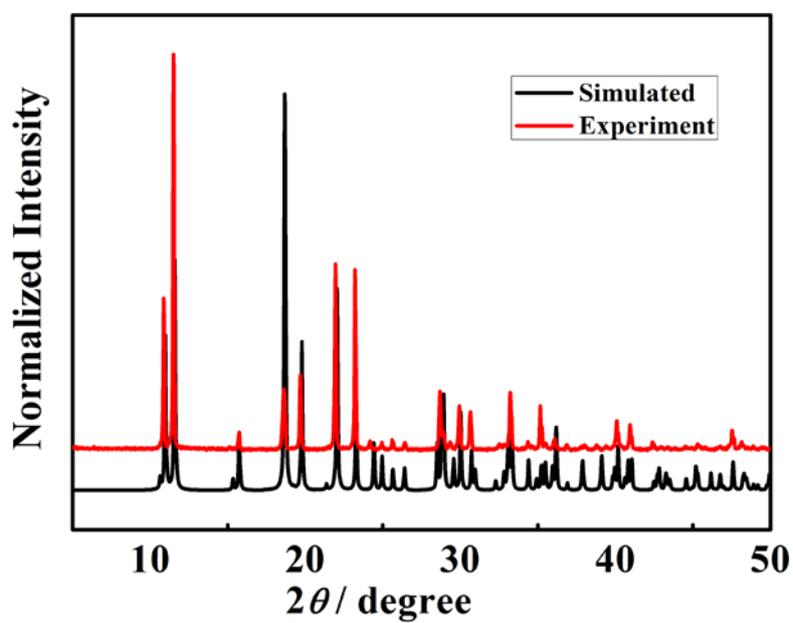


Figure S1. The PXRD spectrum of **2**.

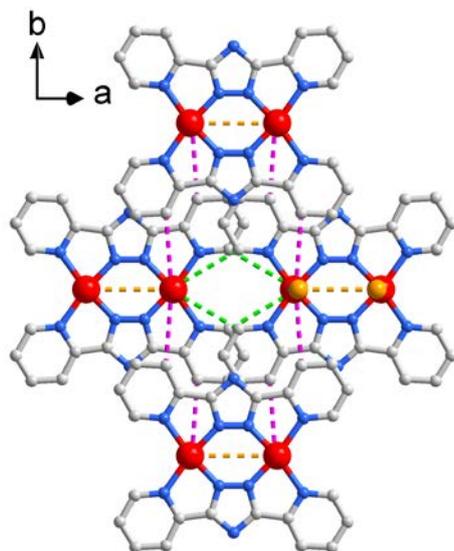
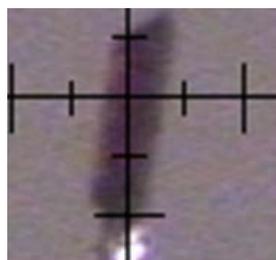
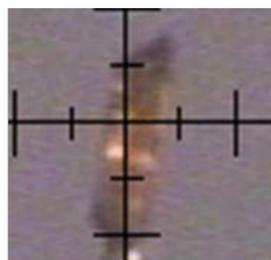


Figure S2. Structural illustrations of **2** at 298 K along the *c* axis: crystal packing of two adjacent 1D chains highlighting the interchains C-H...C (green and purple dashed lines represent 3.659 and 3.529 Å, respectively) interactions and the intrachains Au...Au (orange dashed lines, 3.591 Å) interactions. Hydrogen atoms have been omitted for clarity.



298K



373K

Figure S3. Photographs of single crystal of **2**.

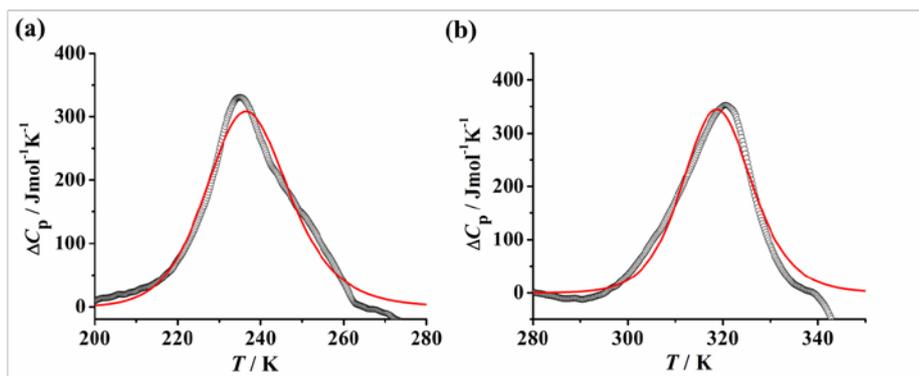


Figure S4. Excess heat capacity associated with the SCO transition for $1 \cdot \text{H}_2\text{O}$ upon warming. The full lines are the best fit to the domain model.

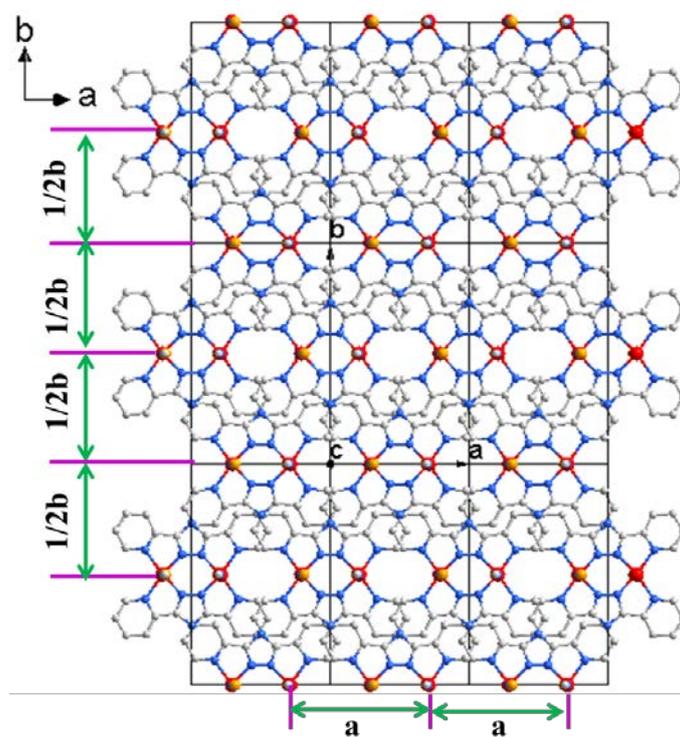


Figure S5. Crystal packing of 2 in the ab plane. The different Fe...Fe projection distances are given for LS 2 .

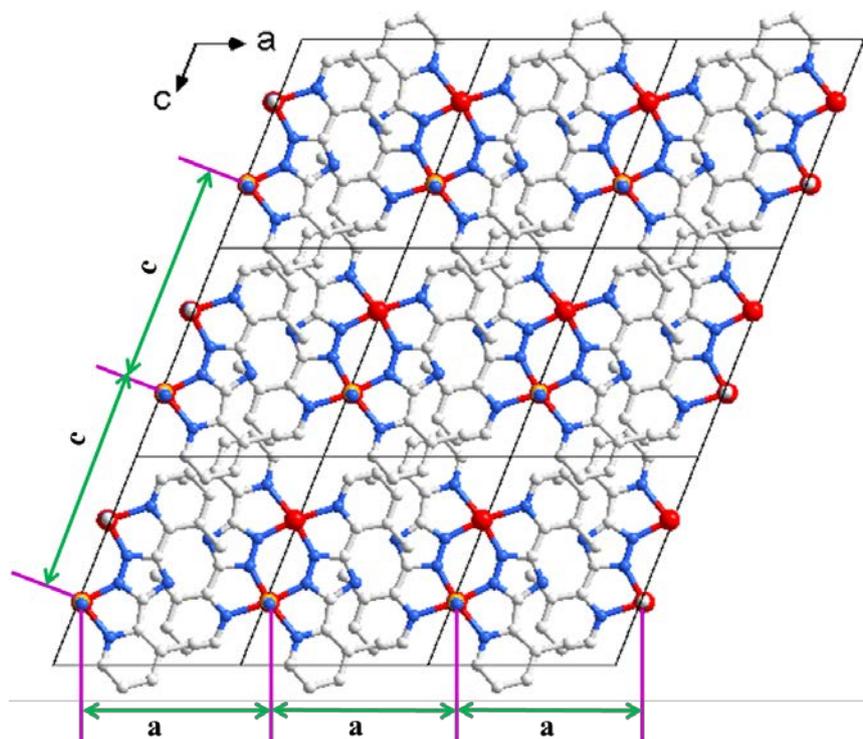


Figure S6. Crystal packing of $1 \cdot \text{H}_2\text{O}$ in the ac plane. The different $\text{Fe} \cdots \text{Fe}$ projection distances are given for LS $1 \cdot \text{H}_2\text{O}$.

Table S1 $\text{Fe} \cdots \text{Fe}$ projection distances observed in the three different crystallographic axes of the solid state structure of **2** and $1 \cdot \text{H}_2\text{O}$, and their variation upon LS \leftrightarrow HS transition

2		Fe...Fe projection distances		
Direction	along a	along b	along c	
LS	11.562	7.656	10.147	
HS	11.604	7.868	10.479	
Variation	0.042	0.212	0.332	
1·H₂O		Fe...Fe projection distances		
Direction	along a	along b	along c	
LS	9.328	10.154	10.849	
HS	9.616	10.473	10.991	
Variation	0.288	0.319	0.142	

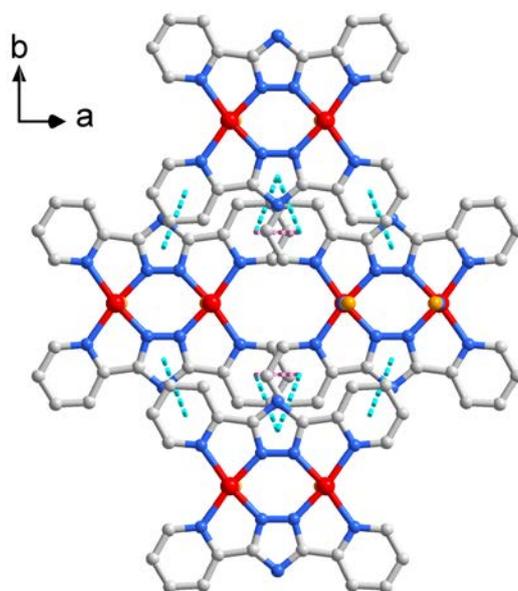


Figure S7. Structural illustrations of **2** along the *c* axis: Crystal packing of two adjacent 1D chains highlighting the interchains offset face-to-face $\pi \cdots \pi$ interactions (turquoise and pink dashed lines represent 4.166 and 3.973 Å, respectively). Hydrogen atoms have been omitted for clarity.

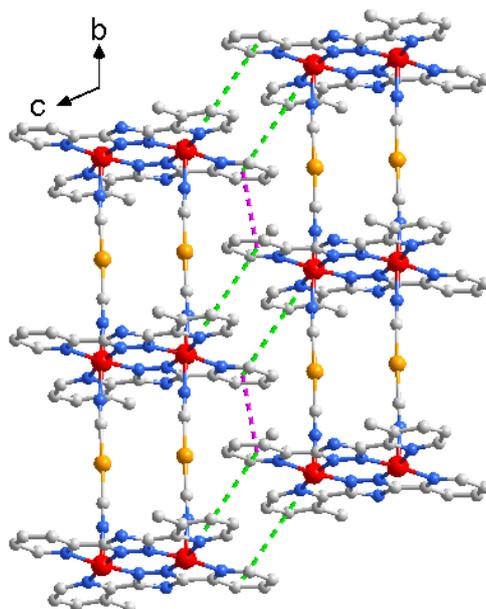


Figure S8. Structural illustrations of **1·H₂O**: Crystal packing of two adjacent 1D chains highlighting the interchains face to face $\pi \cdots \pi$ (green dashed lines, 4.294 Å and purple dashed lines, 3.626 Å) interactions. Hydrogen atoms have been omitted for clarity.