

Supporting Information
for

**Spin-crossover iron(II) long-chain complex with slow spin equilibrium
at low temperature**

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Table S1. Crystal data and structural refinements for complex **1**.

[Fe(H ₂ Bpz ₂) ₂ (C ₉ bpy)]	
<i>T</i> / K	293
Formula	C ₈₀ H ₁₂₀ B ₄ N ₂₀ Fe ₂
MW	1516.88
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> / Å	10.5280(10)
<i>b</i> / Å	22.6959(19)
<i>c</i> / Å	35.720(3)
<i>α</i> / deg	90
<i>β</i> / deg	92.677(7)
<i>γ</i> / deg	90
<i>V</i> / Å ³	8525.6(12)
<i>Z</i>	8
<i>D</i> _{calc} / g/cm ³	1.1786
<i>μ</i> / mm ⁻¹	0.394
Goodness-of-fit on <i>F</i> ²	1.0515
<i>F</i> (000)	3235
<i>R</i> ₁ [<i>I</i> ≥ 2σ(<i>I</i>)]	0.0787
<i>wR</i> ₂ [all data]	0.2067
CCDC no.	2040605

Table S2. Selected bond lengths for complex **1** at 293 K.

Complex 1	
Fe1–N1	2.205(4)
Fe1–N4	2.147(4)
Fe1–N5	2.194(4)
Fe1–N8	2.162(4)
Fe1–N9	2.205(4)
Fe1–N10	2.215(4)
Fe2–N11	2.145(4)
Fe2–N14	2.206(4)
Fe2–N15	2.156(4)
Fe2–N18	2.190(4)
Fe2–N19	2.189(4)
Fe2–N20	2.221(4)

Table S3. Rate Constants $k_{\text{HL}}(T)$ of annealing test at different temperatures.

T / K	$k_{\text{HL}}(T)$
50	8.795E-7
55	2.749E-5
60	3.939E-5
65	6.300E-4

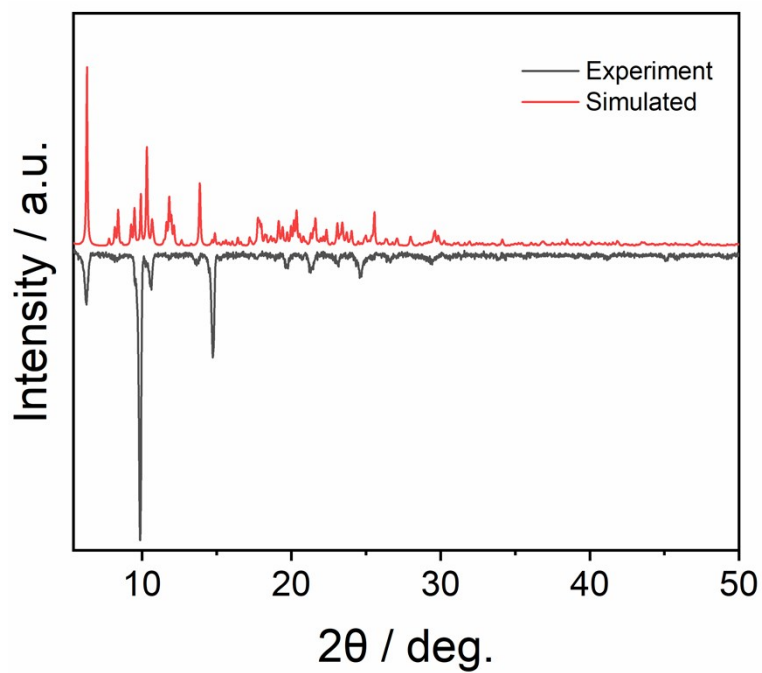


Figure S1. Comparison of the PXR D patterns of **1** measured from polycrystalline sample and simulated based on single-crystal structure.

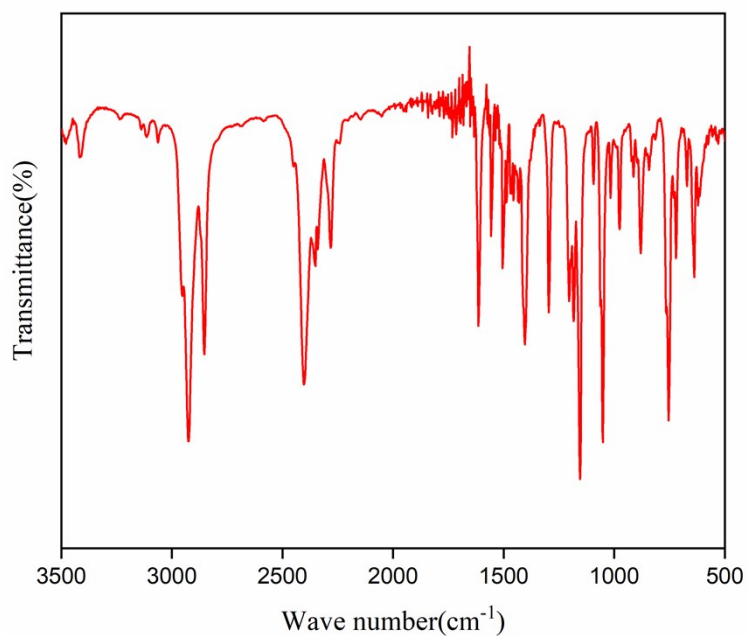


Figure S2. IR spectra of complex **1**. In the FIT-IR spectrum, the characteristic peaks of H_2Bpz_2^- group is around 2400 cm^{-1} and 1153 cm^{-1} . The peaks at 2926 cm^{-1} denotes the vibration of -CH groups.

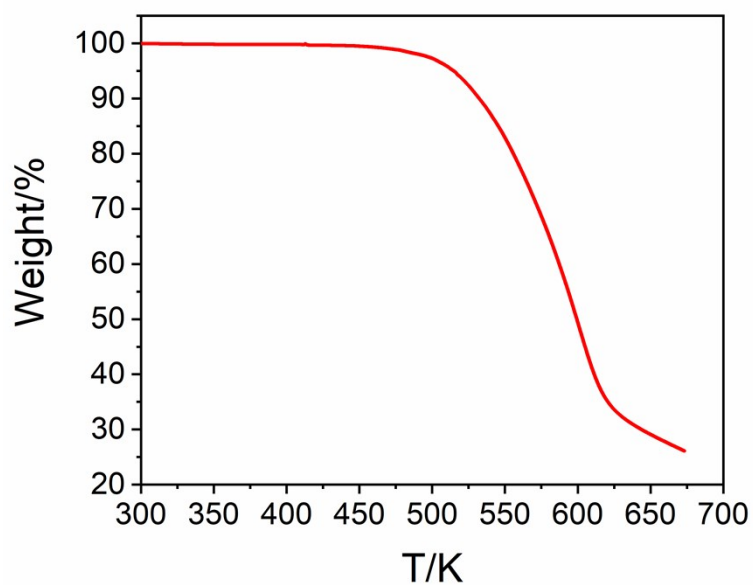


Figure S3. Thermogravimetric data of complex **1**. The thermogravimetric data shows that there is no mass loss at the beginning of heating compound **1**, which confirms that the compound **1** does not contain solvent molecules, and compound **1** will not decompose until heated at 463 K.

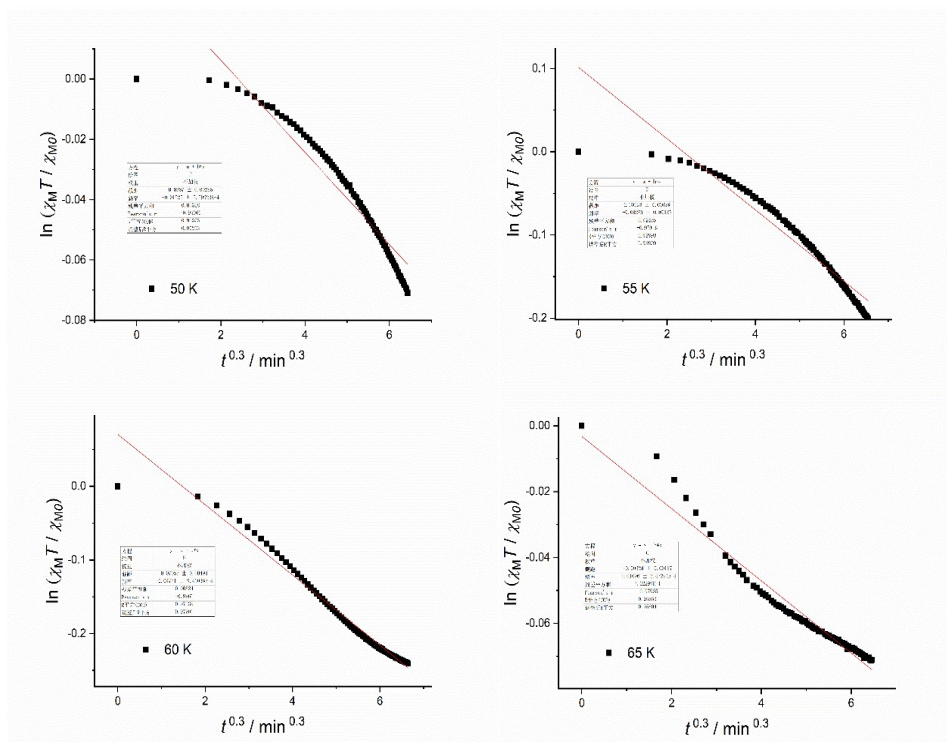


Figure S4. Fitting data of rate constants $k_{HL}(T)$ at different temperatures.