Supporting Information

Lattice water molecules tuned spin-crossover for an iron (Ⅱ) complex with thermal hysteresis

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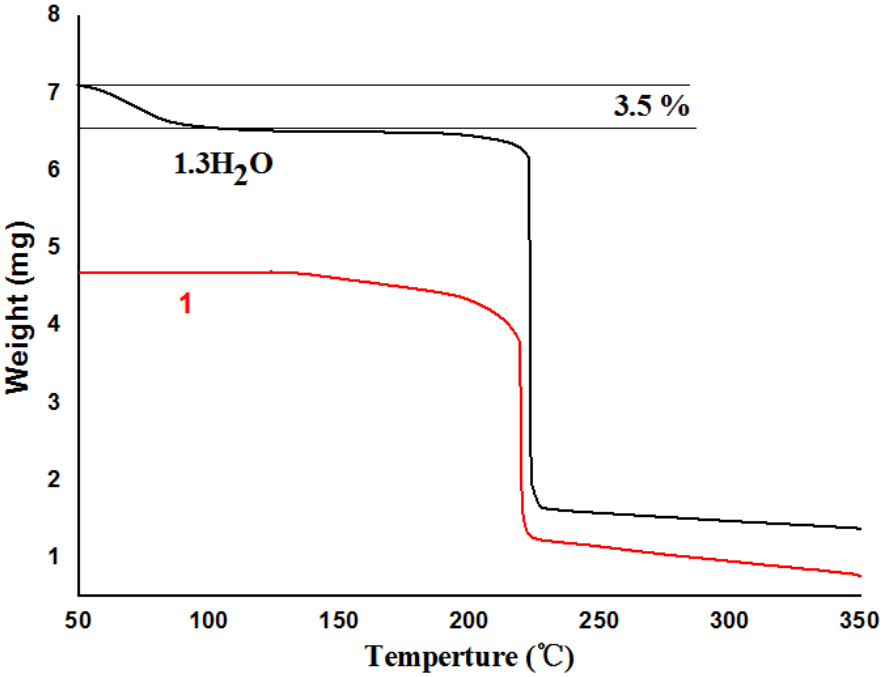

Figure.S1 TGA profiles of complexes **1**·3H_2O and **1** in the 50-350 ℃ region.

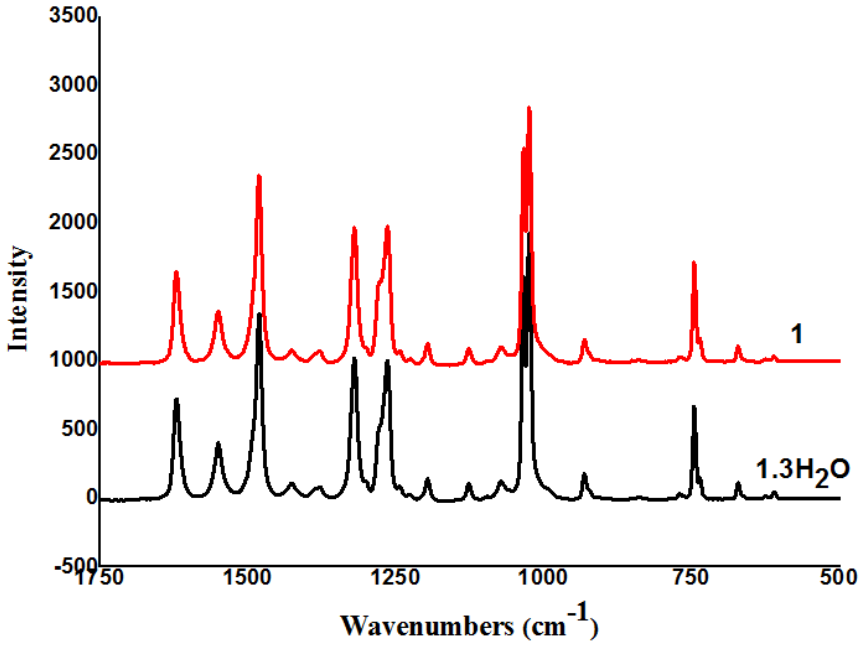

Figure.S2 Raman spectra of complexes **1**·3H_2O and **1** in the 1750-500 cm^{-1} region.

Table S1. The geometrical parameters for the hydrogen bonds in compound **1**·3H_2O at three different temperature

Complex	D–H···A	D–H（Å）	H···A（Å）	D···A（Å）	∠D–H···A(deg)	symmetry operation
300K	C1–H1···N2	0.93	2.57	3.094(5)	116	1-x, y, 3/2-z
	C2–H2···O2	0.93	2.12	2.581(10)	109	
	C12–H12···N3	0.93	2.61	3.099(5)	113	
	C18–H18···N1	0.93	2.56	3.077(6)	115	1-x, y, 3/2-z
240K	C1–H1···O1	0.93	2.6	3.283(15)	131	1-x, y, 1/2-z
	C1–H1···N2	0.93	2.58	3.104(10)	116	1-x, y, 1/2-z
	C4–H4A···O1	0.96	2.59	3.15(16)	117	1/2-x, 1/2-y, -z
	C5–H5···O1	0.93	2.22	3.042(14)	147	1/2-x, 1/2-y, -z
	C12–H12···N3	0.93	2.59	3.078(10)	113	1/2-x, 1/2-y, -z
	C133–H13···N1	0.93	2.57	3.075(10)	114	
130K	C6–H6···N3	0.93	2.6	3.094(7)	114	x, y, 3/2-z
	C9–H9···O1	0.93	2.12	2.969(15)	151	1/2-x, 3/2-y, 2-z
	C13–H13···O1	0.93	2.42	3.088(15)	129	x, y, 3/2-z
	C13–H13···N1	0.93	2.56	3.077(6)	115	x, y, 3/2-z
	C14–H14···N2	0.93	2.58	3.074(6)	114	
	C15–H15A···O1	0.96	2.58	3.395(15)	143	1/2-x, 3/2-y, 2-z

Table S2.The bond angles (º) of the distorted octahedral geometry for complex **1**·3H_2O

	N1-Fe1-N2	N1-Fe1-N3	N1-Fe1-N2A	N2-Fe1-N3	N2-Fe1-N3A
300 K	81.37	95.01	96.01	87.4	95.38
240 K	81.19	95.14	96.21	87.54	95.21
130 K	81.7	87.41	95.73	95.16	175.4

Table S2. Continued

	N3-Fe1-N3A	N1-Fe1-N1A	N2-Fe1-N1A	N1-Fe1-N3A	N2-Fe1-N2A
300 K	80.8	89.3	96	175	176
240 K	80.92	89	96.2	175	176
130 K	81.24	176	95.7	95.3	88.6

Table S3. Summary of main contacts contribute to Hirshfeld surfaces (%) in the three forms of complex **1**·3H_2O.

	N-H	C-C	C-H	H-H	H-O	C-O	H-Cl
300K	0.8	0.2	23.5	47.8	24.9	1.7	0.6
240K	0.7	0.3	24.5	50.9	21.2	1.6	0.1
130K	0.7	0.4	25.3	51.6	20.1	1	0.1

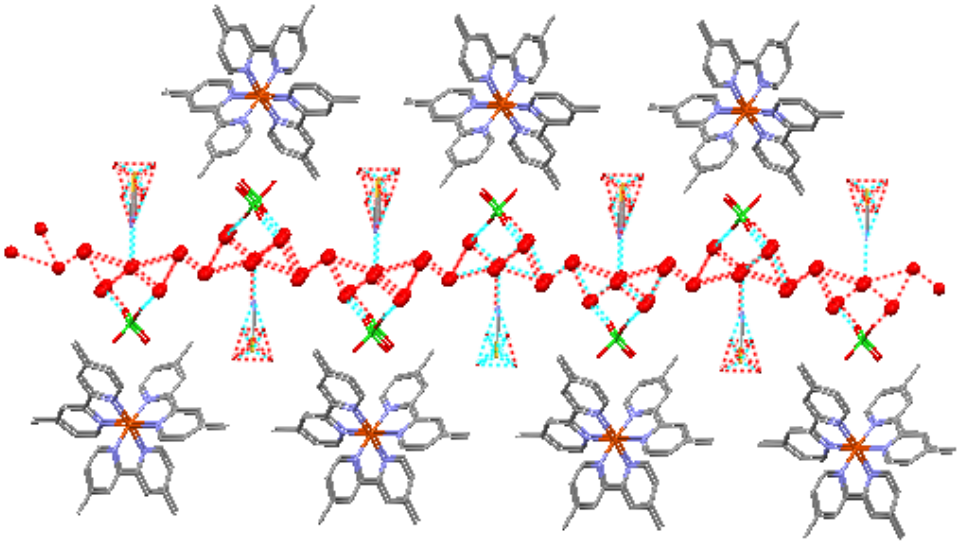

Fig.S3. 3D packing diagrams of complex **1**·3H_2O along the crystallographic *a*-axes, hydrogen atoms are omitted for clarity.

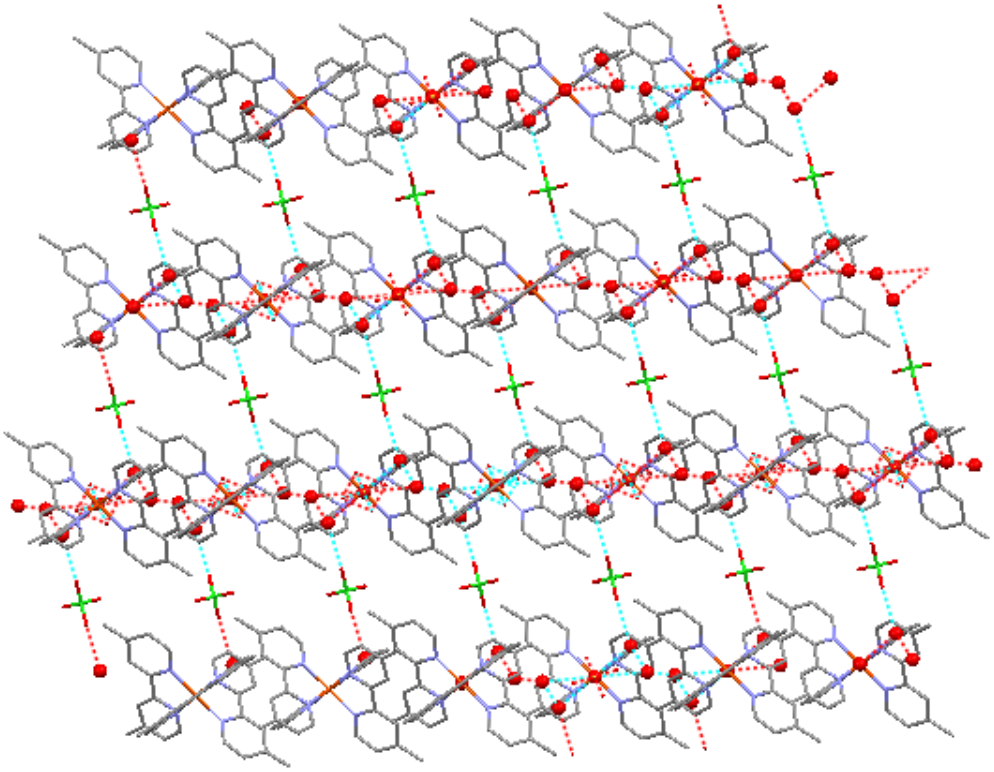

Fig.S4. 3D packing diagrams of complex **1**·3H_2O along the crystallographic *b*-axes, hydrogen atoms are omitted for clarity.

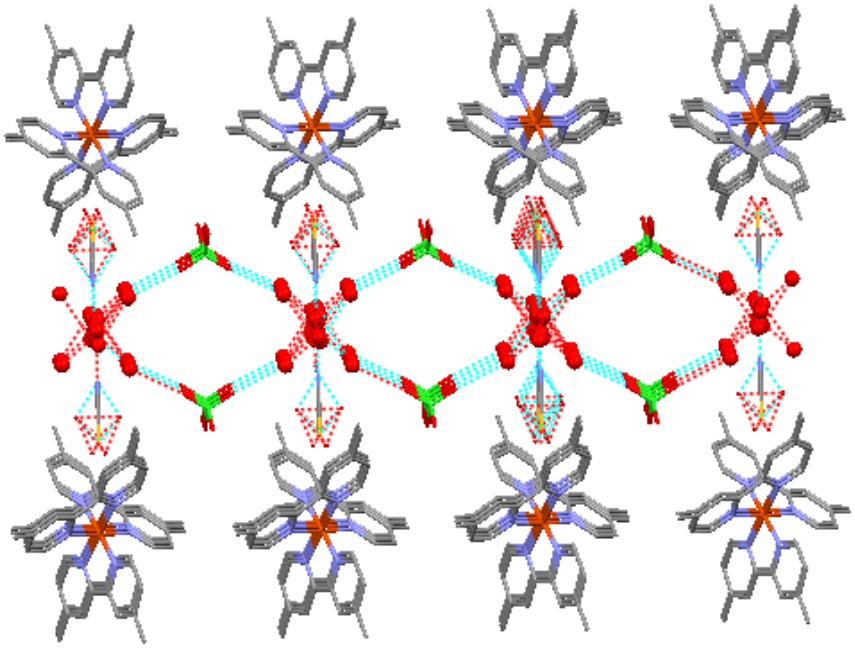

Fig.S5. 3D packing diagrams of complex **1**·3H_2O along the crystallographic *c*-axes, hydrogen atoms are omitted for clarity.

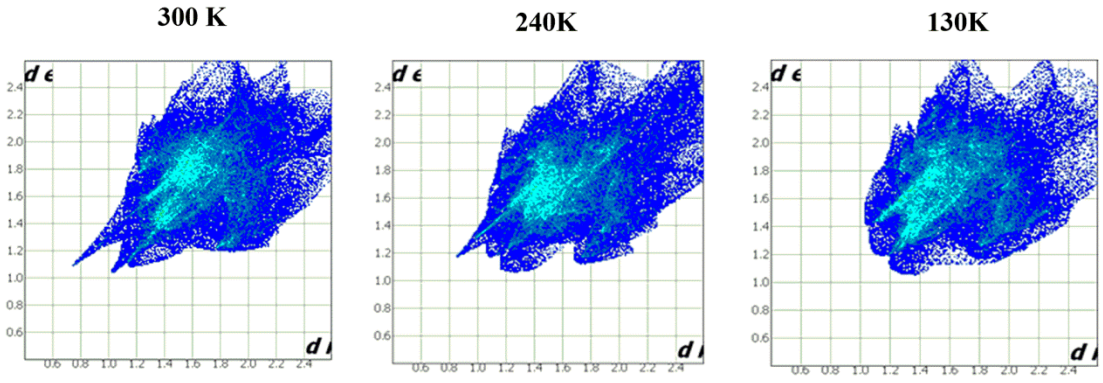

Fig.S6. 2D fingerprint plots of complex **1**·3H_2O at three different temperatures