

Electronic Supplementary Material (ESI) for *Inorganic Chemistry Frontiers*

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## **Structural and Magnetic Tuning from Field-Induced Single-Ion Magnet to Single-Chain Magnet by Anions†**

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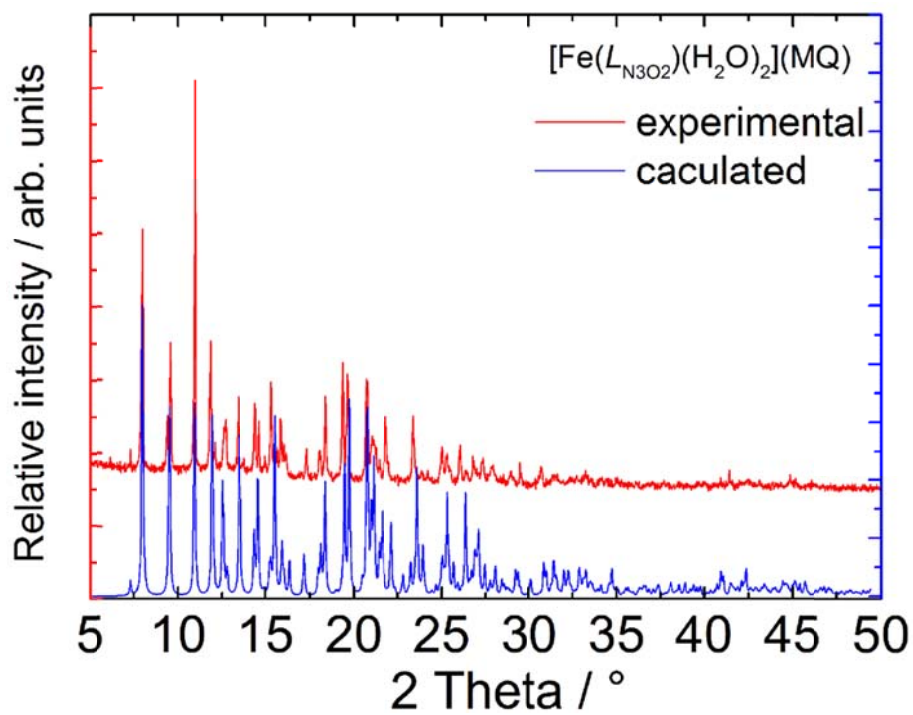
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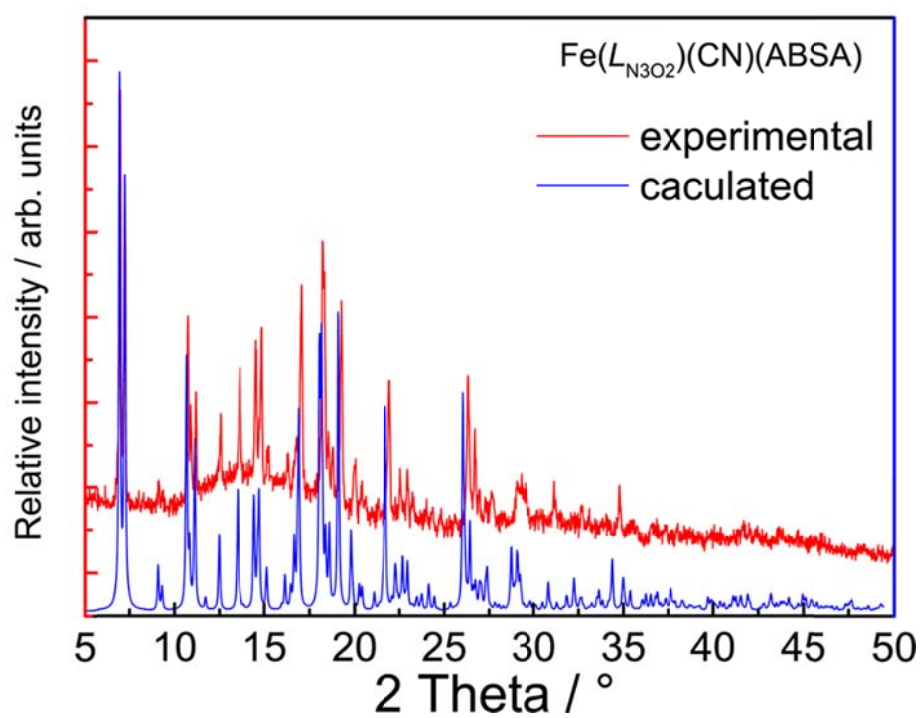
Supporting Information

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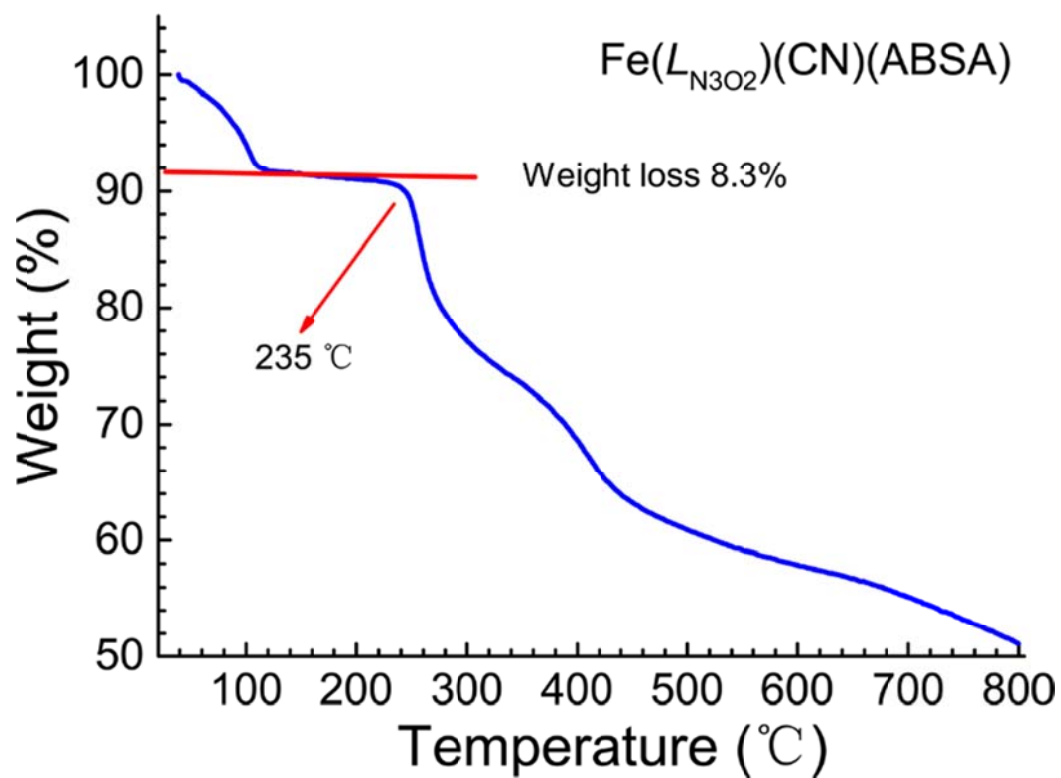
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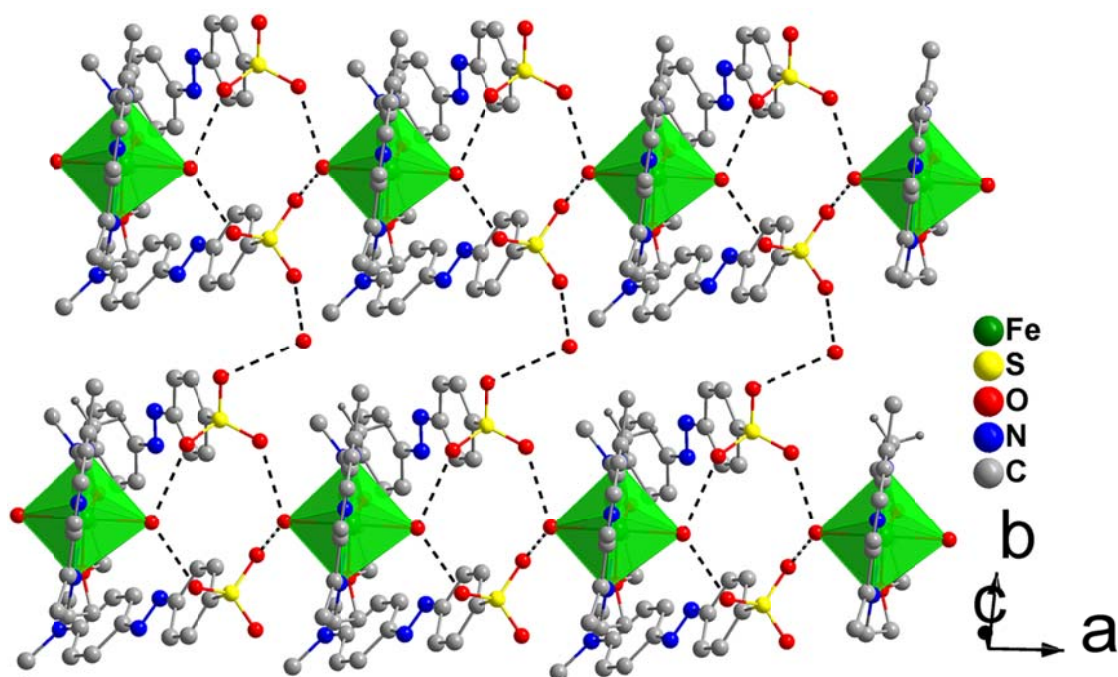
**Fig. S1** Experimental and calculated XRPD pattern for **1**.



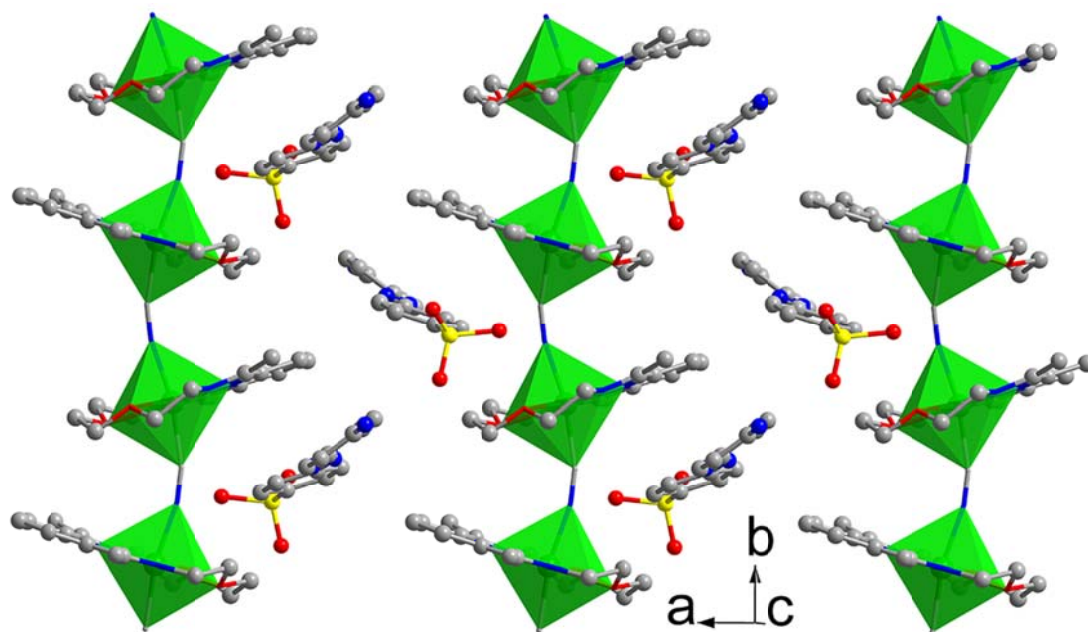
**Fig. S2** Experimental and calculated XRPD pattern for **2**.



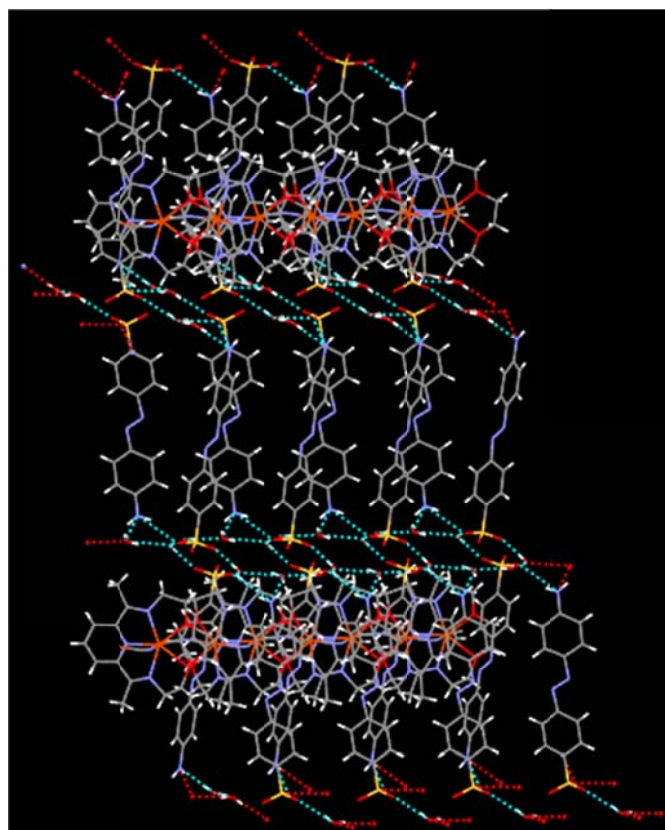
**Fig. S3** TG curve of compound **2** at a rate of 10 K/min under a  $\text{N}_2$  atmosphere.



**Fig. S4** The 2D supramolecular layer of **1** along the  $ab$  plane.



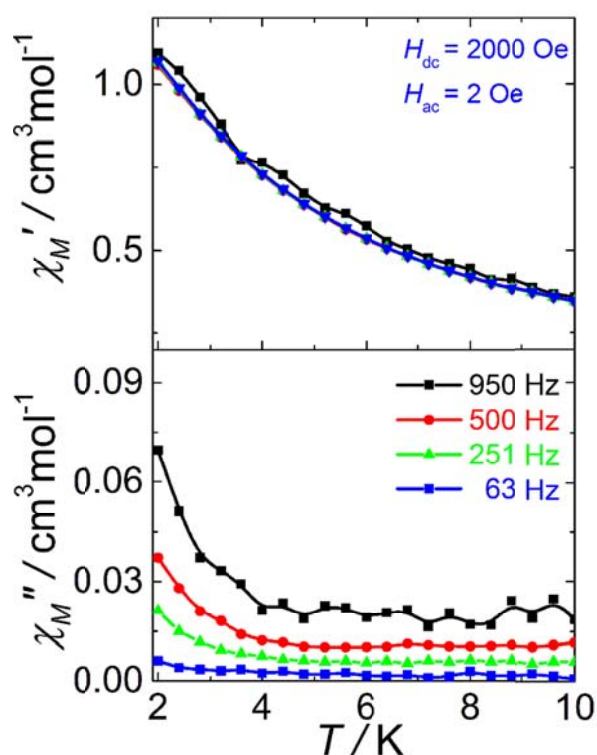
**Fig. S5** The side view of the packing structure of **2**.

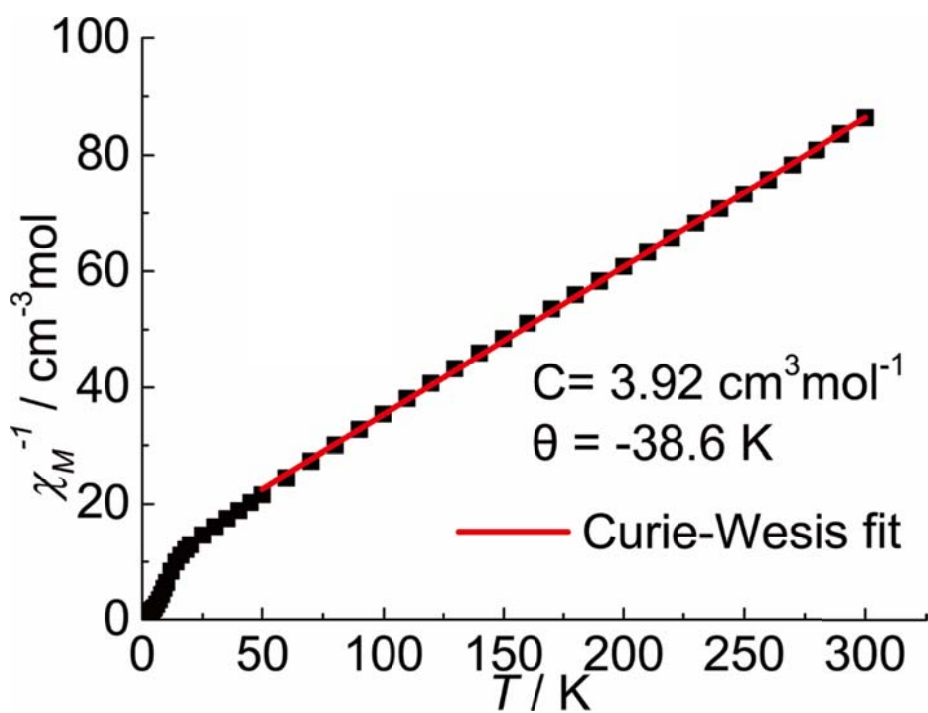


**Fig. S6** The abundant hydrogen bonds in **2**.

**Table S1** Selected bond lengths (Å) and angles (°) for **1** and **2**

1					
Fe1-N1	2.136(4)	Fe1-O1	2.266(4)	Fe1-O3	2.143(4)
Fe1-N2	2.170(4)	Fe1-O2	2.276(3)	Fe1-O4	2.126(4)
Fe1-N3	2.215(4)				
O4-Fe1-O3	174.68(14)	O4-Fe1-N2	90.50(15)	O4-Fe1-N1	96.97(16)
N1-Fe1-O3	88.32(16)	O3-Fe1-O1	93.14(14)	O3-Fe1-N3	91.90(16)
2					
Fe1-N1	2.114(3)	Fe1-C28#1	2.137(2)	Fe1-O1	2.266(4)
Fe1-N2	2.180(4)	Fe1-N4	2.149(3)	Fe1-O2	2.276(3)
Fe1-N3	2.184(3)				
N1-Fe1-C28#1	99.41(10)	C28#1-Fe1-N4	168.24(11)	C28#1-Fe1-N2	92.85(10)
C28-N4-Fe1	166.5(3)	N4-C28-Fe1#2	165.7(3)		
#1 -x,y-1/2,-z+1/2    #2 -x,y+1/2,-z+1/2					

**Fig. S7** Variable-temperature ac magnetic susceptibility data for **1** measured under a 2 kOe dc field.



**Fig. S8** The  $\chi_M^{-1}$  vs.  $T$  plot and the Curie-Weiss fit of **2**.

**Table S2** Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **2** according to the generalized Debye model.

$T / \text{K}$	$\chi_S / \text{cm}^3 \text{mol}^{-1} \text{K}$	$\chi_T / \text{cm}^3 \text{mol}^{-1} \text{K}$	$\tau / \text{s}$	$\alpha$
1.80	0.27534	0.65634	0.00188	0.41597
1.85	0.25202	0.64220	0.00116	0.44452
1.90	0.23103	0.62331	0.00068	0.44063
1.95	0.25627	0.61006	0.00052	0.40704
2.00	0.25092	0.60343	0.00044	0.44874
2.05	0.25000	0.58398	0.00029	0.38360
2.10	0.29163	0.57743	0.00022	0.41622