Supporting Information for

Dynamic magnetism of an iron(II)-chlorido spin chain and its hexametallic segment

Lei Qin,[a,#] Zhong Zhang,[a,#] Zhiping Zheng,[a,c] Manfred Speldrich,[b] Paul Kögerler,[b] Wei Xue,[d] Bao-Ying Wang,[d] Xiao-Ming Chen[d] and Yan-Zhen Zheng,*[a]

[a] *Center for Applied Chemical Research, Frontier Institute of Chemistry, Frontier Institute of Science and Technology, and State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710054, China.*

[b]*Institute of Inorganic Chemistry, RWTH Aachen University, D-52074 Aachen, Germany.*

[c]*Department of Chemistry, The University of Arizona, Tucson, Arizona 85721, USA.*

[d] *MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry & Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China.*

[#] These authors contribute equally in this work.

Corresponding Email to YZZ: zheng.yanzhen@mail.xjtu.edu.cn

Table S1 Experimental data for complex **2.**

	2
Empirical formula	$C_{72}H_{48}Cl_{12}Fe_6N_{12}$
Colour/shape	Red/block
Formula weight	1841.72
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	
a(Å)	10.0016(11)
b(Å)	10.2378(11)
c(Å)	19.241(2)
α(º)	80.0380(10)
β(º)	84.4460(10)
γ(º)	61.9170(10)
Volume(Å^3)	1711.7(3)
Z	1
$D_{calc.}$ (Mg·m^{-3})	1.787
Absorption coefficient(mm^{-1})	1.762
F(000)	924
Crystal size	0.31 x 0.24 x 0.20
θ range for data collection (º)	2.15 - 27.64
Reflections collected	39581
Unique reflections	7921 [R(int) = 0.0183]
Completeness to *θ* = 25.01	99.3 %
Absorption correction	Semi-empirical
Max. and min. transmission	0.7194 and 0.6111
Data / restraints / parameters	7921 / 0 / 460
Goodness-of-fit on F^2	1.147
R indices [$I>2\sigma(I)$]	R_1 = 0.0354, wR_2 = 0.0866
R indices (all data)	R_1 = 0.0393, wR_2 = 0.0882
Largest diff. features (e Å^{-3})	0.925 and -0.381
CCDC	959874

Table S2 The selected bond lengths (Å) and angles (º) for complex **2.**

For **2**

Fe(1)-N(2)	2.188(2)	Fe(2)-Cl(3)	2.5533(7)
Fe(1)-N(1)	2.200(2)	Fe(2)-Cl(5)	2.5889(7)
Fe(1)-Cl(1)	2.3186(7)	Fe(3)-N(6)	2.1669(19)
Fe(1)-Cl(3)	2.4224(7)	Fe(3)-N(5)	2.181(2)
Fe(1)-Cl(2)	2.4372(7)	Fe(3)-Cl(6)	2.4209(7)
Fe(2)-N(4)	2.165(2)	Fe(3)-Cl(5)	2.4225(7)
Fe(2)-N(3)	2.174(2)	Fe(3)-Cl(6)#1	2.6003(7)
Fe(2)-Cl(4)	2.4082(7)	Fe(3)-Cl(4)	2.6200(7)
Fe(2)-Cl(2)	2.4742(7)	Cl(6)-Fe(3)#1	2.6004(7)
N(2)-Fe(1)-N(1)	75.41(8)	N(2)-Fe(1)-Cl(1)	150.58(6)
N(1)-Fe(1)-Cl(1)	92.04(6)	N(2)-Fe(1)-Cl(3)	90.67(6)
N(1)-Fe(1)-Cl(3)	165.83(6)	Cl(1)-Fe(1)-Cl(3)	99.12(2)
N(2)-Fe(1)-Cl(2)	99.77(6)	N(1)-Fe(1)-Cl(2)	94.71(6)
Cl(1)-Fe(1)-Cl(2)	107.81(3)	Cl(3)-Fe(1)-Cl(2)	90.18(2)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+2

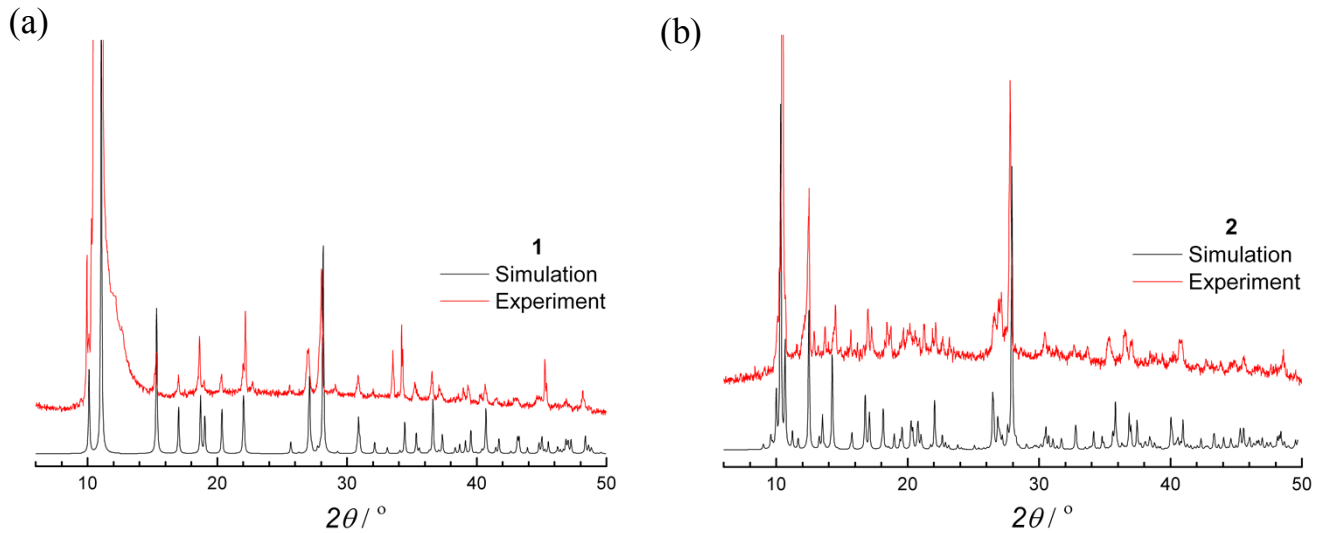

Figure S1 The powder X-ray diffractions of compounds **1** and **2**.

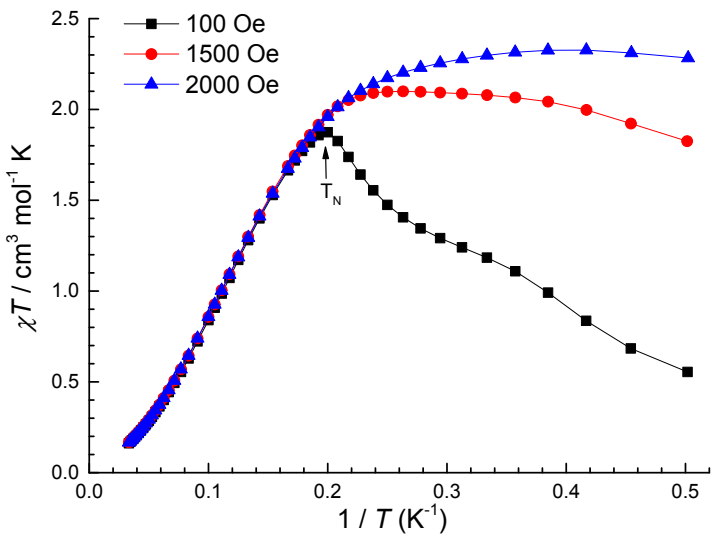

Figure S2 The χT vs. T^{-1} plots under different fields of **1**.