Electronic Supplementary Information

for

An iron(III)-centred ferric wheel Fe⊂{Fe_6} with a siloxane-based *bis*-salicylidene Schiff base

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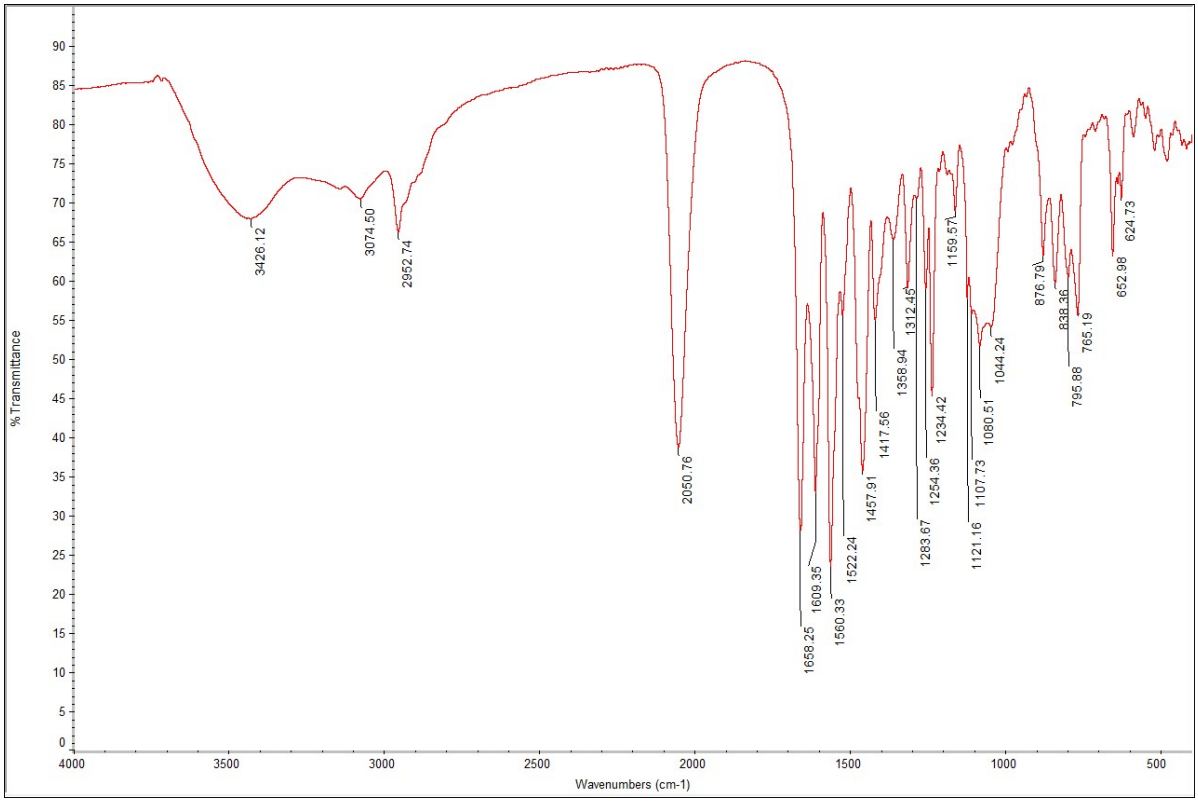

Fig. S1. FT-IR spectrum of $[Fe_7(H_2L)_6(NCS)_6]\cdot 10H_2O$ (**1**) in KBr.

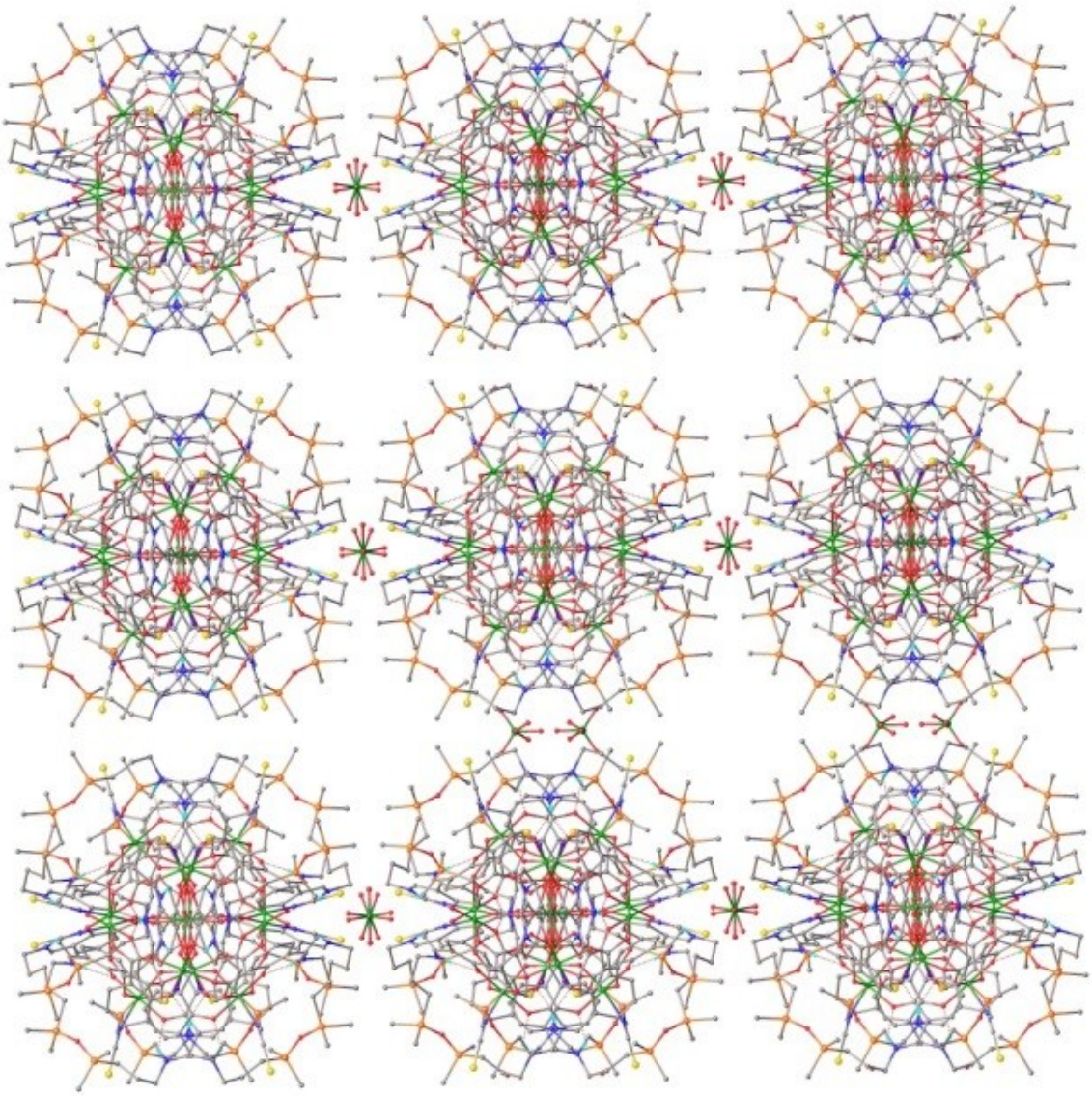

Figure S2. Crystal packing of $[Fe_7(H_2L)_6(NCS)_6]\cdot 10H_2O$ (**1**).

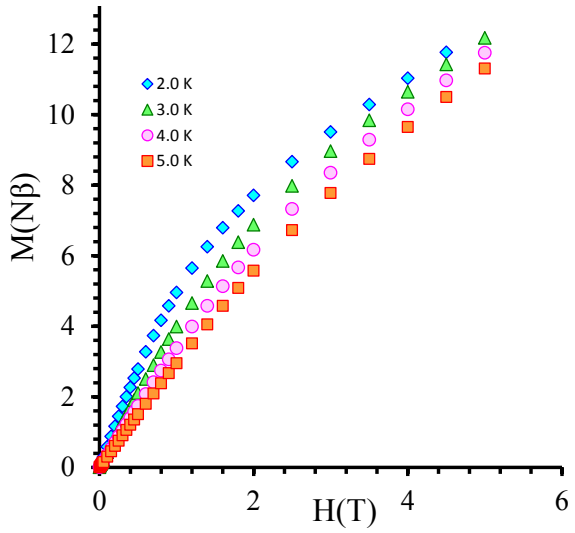

Figure S3. Magnetisation curves for **1** at 2, 3, 4, and 5 K.

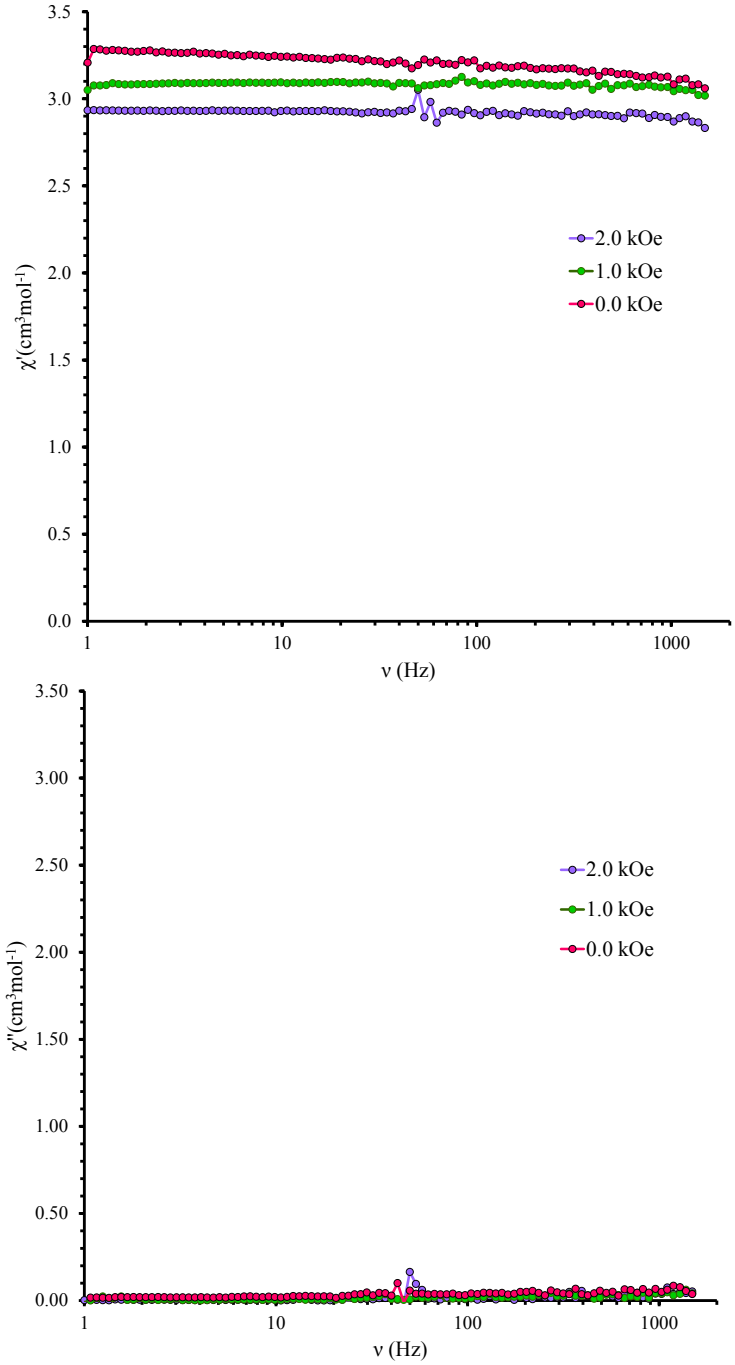

Figure S4. Frequency dependence of the in-phase (top) and out-of-phase (bottom) components of the *ac* magnetic susceptibility data for **1.** Data collected with 3.0 Oe *ac* oscillated field at 2 K under indicated *dc* fields (0.0, 1.0 , 2.0 kOe).

Table S1. Crystallographic data, details of data collection and structure refinement parameters for **1**.*

Empirical formula	$C_{162}H_{156}Fe_7Cl_3N_{18}O_{54}S_6Si_{12}$
Formula weight	4245.78
Temperature/K	173.0(1)
Crystal system	cubic
Space group	*Ia*-3
a/Å	41.2312(7)
V/Å^3	70094(4)
Z	8
D_{calc}/mg/mm^3	0.805
μ/mm^{-1}	0.427
Crystal size/mm^3	0.1 × 0.1 × 0.1
θ_{min}, θ_{max}(°)	3.12 to 55.54
Reflections collected	33398
Independent reflections	8301 [R_{int}= 0.2047]
Data/restraints/parameters	8301/0/400
GOF[c]	0.821
R_1[a]($I>2\sigma(I)$)	0.0759
wR_2[b](all data)	0.1421
Largest diff. peak/hole/e Å^{-3}	0.38/-0.26

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b]$wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. [c] GOF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined.

*The (very low) crystal density, as well as μ and formula weight, were calculated without the masked solvent.

Table S2. Bond lengths (Å) and bond angles (°) in **1**.

Fe1-O1	1.990(3)	N2-C8	1.269(7)
Fe2-O2	1.992(3)	N2-C9	1.469(6)
Fe2-O3	2.006(3)	N3-C27	1.142(6)
Fe2-O4	1.959(4)	C1-C2	1.483(7)
Fe2-O5	2.026(4)	C2-C3	1.384(7)
Fe2-O6^{1}	1.997(4)	C2-C7	1.402(7)
Fe2-N3	2.019(5)	C3-C4	1.366(7)
S1-C27	1.619(6)	C4-C5	1.375(7)
Si1-O7	1.599(6)	C5-C6	1.411(7)
Si1-C14	1.753(9)	C6-C7	1.417(7)
Si1-C15	1.883(7)	C6-C8	1.480(7)
Si1-C16	1.890(7)	C9-C10	1.517(8)
Si2-O7	1.528(6)	C10-C11	1.497(7)
Si2-C11	1.865(6)	C16-C17	1.406(8)
Si2-C12	1.834(9)	C17-C18	1.500(7)
Si2-C13	1.843(7)	C19-C20	1.417(7)
O1-C1	1.241(6)	C20-C21	1.420(7)
O2-C1	1.275(6)	C20-C25	1.390(7)
O3-C7	1.299(6)	C21-C22	1.431(7)
O4-C21	1.285(6)	C22-C23	1.394(7)
O5-C26	1.250(6)	C22-C26	1.485(7)
O6-C26	1.275(6)	C23-C24	1.385(7)
N1-C18	1.469(6)	C24-C25	1.342(8)
N1-C19	1.281(6)		

O1^{1}-Fe1-O1	96.18(14)	C27-N3-Fe2	162.3(5)
O1^{5}-Fe1-O1	180	O1-C1-O2	123.2(5)
O1^{3}-Fe1-O1	83.83(14)	O1-C1-C2	119.2(5)
O1^{2}-Fe1-O1	83.82(14)	O2-C1-C2	117.6(5)
O1^{4}-Fe1-O1	96.17(14)	C3-C2-C1	117.2(5)
O2-Fe2-O3	85.05(14)	C3-C2-C7	119.4(5)
O2-Fe2-O5	85.18(15)	C7-C2-C1	123.3(5)
O2-Fe2-O6^{1}	89.49(15)	C4-C3-C2	123.2(5)
O2-Fe2-N3	169.92(16)	C3-C4-C5	119.3(5)
O3-Fe2-O5	92.25(14)	C4-C5-C6	119.2(6)
O3-Fe2-N3	85.19(16)	C5-C6-C7	121.4(6)
O4-Fe2-O2	94.93(14)	C5-C6-C8	119.0(6)
O4-Fe2-O3	178.98(15)	C7-C6-C8	119.5(5)
O4-Fe2-O5	86.73(15)	O3-C7-C2	124.1(5)
O4-Fe2-O6^{1}	88.95(14)	O3-C7-C6	118.5(5)
O4-Fe2-N3	94.78(16)	C2-C7-C6	117.4(5)
O6^{1}-Fe2-O3	92.07(14)	N2-C8-C6	123.3(6)
O6^{1}-Fe2-O5	172.83(15)	N2-C9-C10	107.7(5)
O6^{1}-Fe2-N3	93.38(17)	C11-C10-C9	115.0(6)
N3-Fe2-O5	92.69(17)	C10-C11-Si2	115.4(5)

O7-Si1-C14	111.9(4)	C17-C16-Si1	118.5(6)
O7-Si1-C15	112.8(4)	C16-C17-C18	118.0(6)
O7-Si1-C16	108.4(4)	N1-C18-C17	109.9(5)
C14-Si1-C15	104.3(5)	N1-C19-C20	126.3(6)
C14-Si1-C16	109.7(4)	C19-C20-C21	120.3(6)
C15-Si1-C16	109.7(4)	C25-C20-C19	120.0(6)
O7-Si2-C11	107.6(3)	C25-C20-C21	119.6(6)
O7-Si2-C12	108.5(4)	O4-C21-C20	118.2(6)
O7-Si2-C13	111.3(3)	O4-C21-C22	123.4(6)
C12-Si2-C11	109.8(4)	C20-C21-C22	118.4(6)
C13-Si2-C11	108.4(4)	C21-C22-C26	122.1(6)
C13-Si2-C12	111.2(4)	C23-C22-C21	118.9(6)
C1-O1-Fe1	130.0(3)	C23-C22-C26	119.0(6)
C1-O2-Fe2	132.7(4)	C24-C23-C22	120.5(7)
C7-O3-Fe2	130.4(4)	C25-C24-C23	121.2(7)
C21-O4-Fe2	132.3(4)	C24-C25-C20	121.2(7)
C26-O5-Fe2	131.3(4)	O5-C26-O6	122.5(6)
C26-O6-Fe2[4]	130.6(3)	O5-C26-C22	121.6(6)
Si2-O7-Si1	151.0(5)	O6-C26-C22	115.6(6)
C19-N1-C18	122.2(5)	N3-C27-S1	179.0(7)
C8-N2-C9	119.1(6)		

Symmetry codes: [1]*z*, *x*, y; [2]*y*, *z*, *x*; [3]0.5 – *z*, 0.5 – *x*, 0.5 – *y*; [4]0.5 – *x*, 0.5 – *y*, 0.5 – *z*; [5]0.5 – *y*, 0.5 – *z*, 0.5 – *x*.