Electronic Supplementary Information for Dalton Transactions

Supplementary materials

Supramolecular metallomacrocycles based on trans-dicyanoferrite(III) building blocks: synthesis, crystal structure and magnetic properties

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Table S1. Crystallographic data for complexes **2** and **3**

	2	**3**
formula	$C_{38}H_{34}FeMnN_8O_6$	$C_{38}H_{33}ClFeMnN_8O_6$
Fw	810.53	843.96
T/K	173(2)	293(2)
crystal system	tetragonal	tetragonal
space group	P-42_1c	P-42_1c
a/Å	23.047(3)	23.1615(1)
b/Å	23.047(3)	23.1615(1)
c/Å	15.195(3)	15.1805(1)
□/deg	90	90
□deg	90	90
□/deg	90	90
V/Å^3	8071(2)	8143.66(7)
Z	8	8
□$_{calcd}$/g cm^{-1}	1.332	1.377
F(000)	3336	3464
Reflections collected	14280	7548
R*int*	0.0395	0.0000
Reflections [I > 2σ(I)]□	5994	4780
Goodness-of-fit on F^2	1.012	1.007
data/restraints/params	7099/38/482	7548/0/507
R1[I > 2σ(I)]	0.0846	0.0607
wR2(all data)	0.2367	0.1732
Largest diff. peak , hole (e Å^{-3})	0.914, -0.510	0.577, -0.404
CCDC number	699871	699872

Table S2. Selected bond distances (Å) and bond angles (deg) for complexes **2** and **3**

	2	**3**
Mn(1)-N(1)	2.272(3)	2.268(4)
Mn(1)-O(5)/O(1W)	2.297(2)	2.316(3)
Mn(1)-N(7)	2.052(3)	2.035(4)
Mn(1)-N(8)	2.047(3)	2.043(4)
Mn(1)-O(3)	1.901(3)	1.886(3)
Mn(1)-O(4)	1.896(2)	1.889(3)
Fe(1)-C(1)	2.000(3)	1.987(4)
Fe(1)-C(2)	1.961(4)	1.956(4)
Fe(1)---Mn(1)	5.353(2)	5.319(1)
Fe(1)---Mn(1)’	7.044(2)	7.048(1)
Mn(1)-N(1)-C(1)	166.7(3)	166.8(4)

Table S3. Hydrogen bonding interaction within the supramolecular clusters in complexes **2** and **3**

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
2 O1W-H1A	0.815	2.030	167.16	2.831(4)	N2#2
3 O5-H5	0.856	2.006	160.12	2.825(4)	N2#3

symmetry operations: #2 -y+1, x, -z; #3 y-1, -x+1, -z.

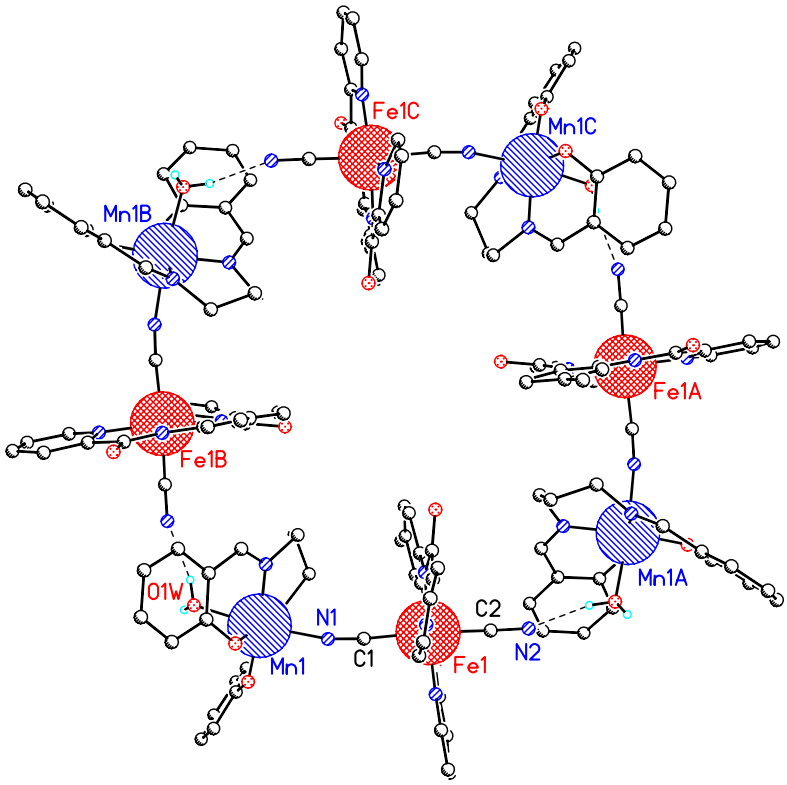

Fig. S1. Structure of a supramolecular square formed from four dinuclear MnFe units of complex **2**. Hydrogen atoms are omitted for clarity.

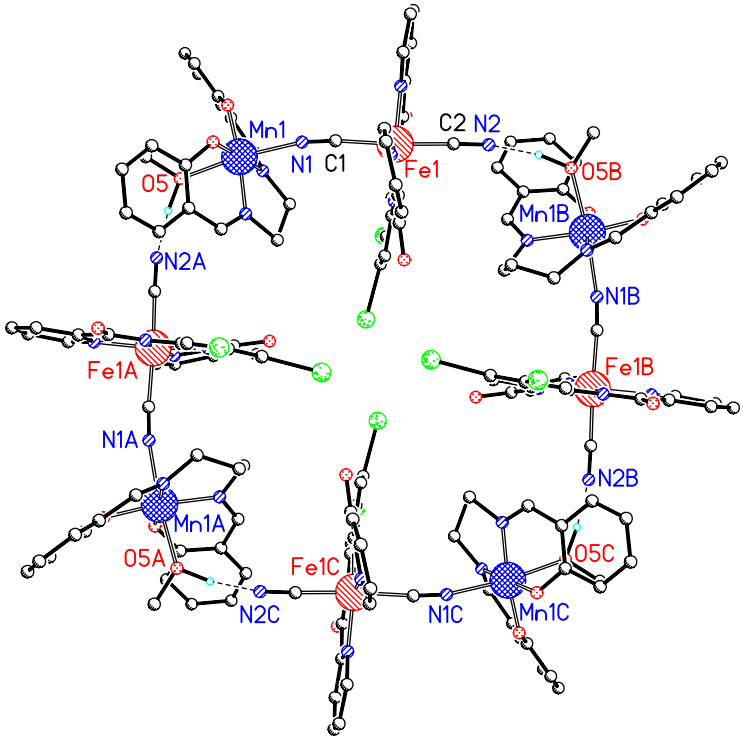

Fig. S2. Structure of a supramolecular square formed from four dinuclear MnFe units of complex **3**. Hydrogen atoms are omitted for clarity.

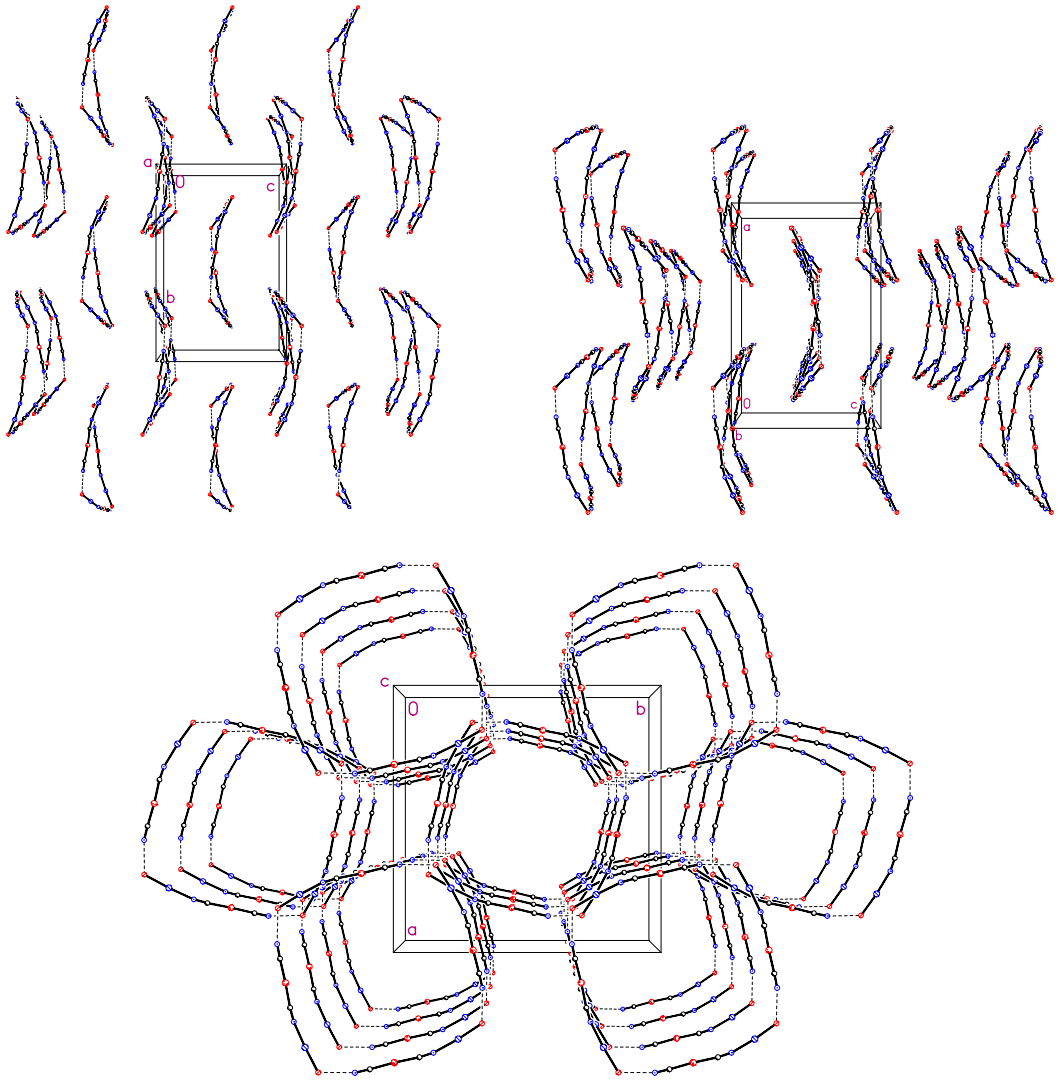

Fig. S3. Packing diagram of the supramolecular macrocycles along the *a, b*, and *c* axes for complex **1**.

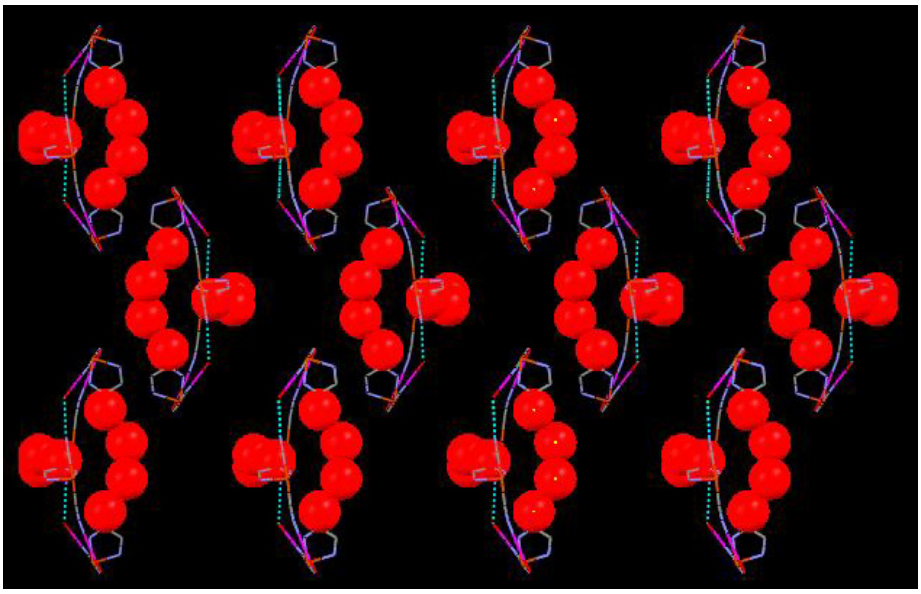

Fig. S4. Projection showing the crystallization water molecules (red balls) around the supramolecular macrocycles in complex **1.**

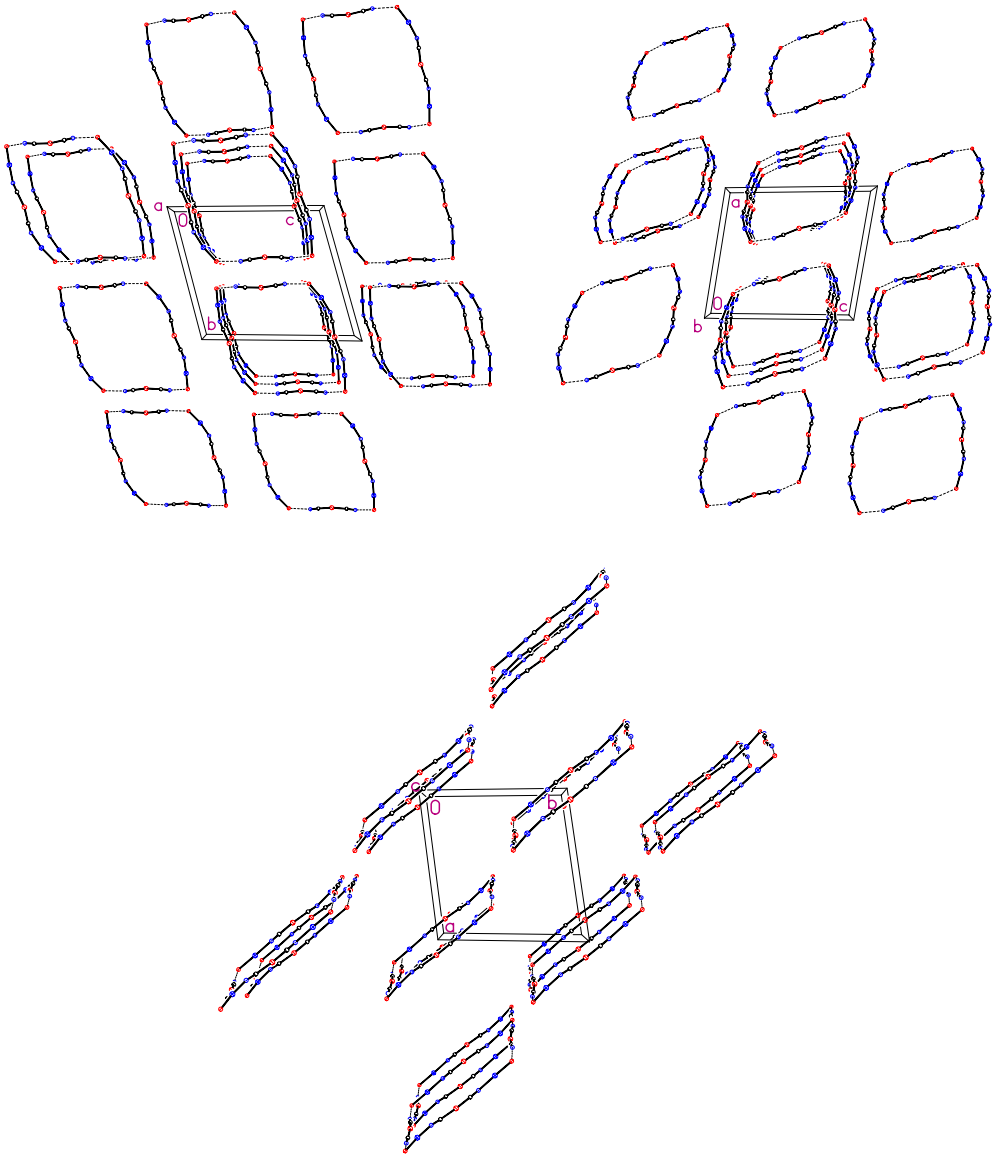

Fig. S5. Packing diagram of the supramolecular metallomacrocycles along the *a, b*, and *c* axes in complex **4.**

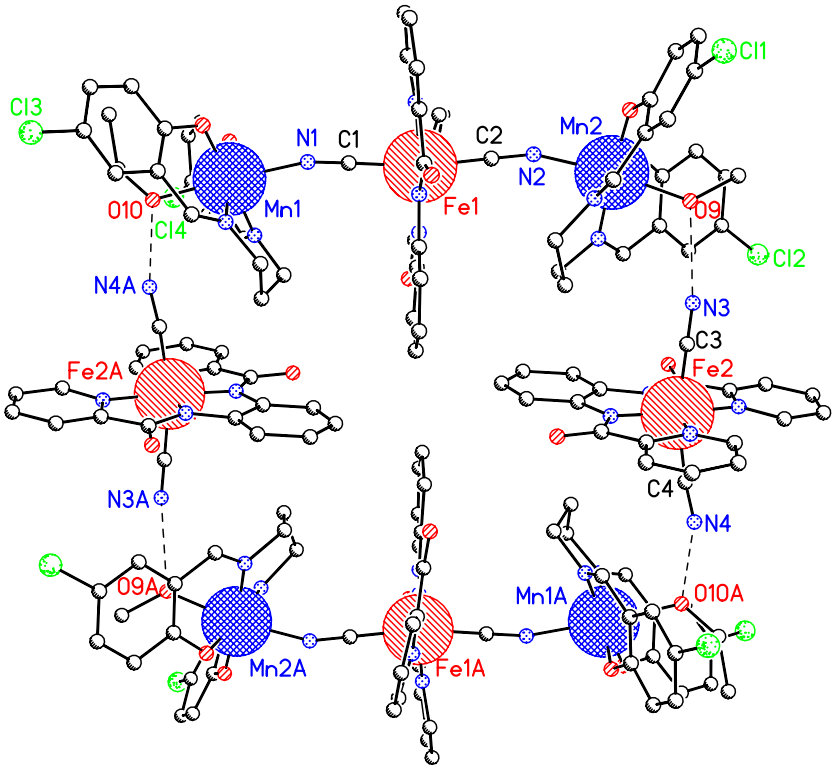

Fig. S6. Structure of a supramolecular rectangle formed from two triinuclear Mn_2Fe and two $[Fe(bpb)(CN)_2]^-$ units of complex **5**. Hydrogen atoms are omitted for clarity.

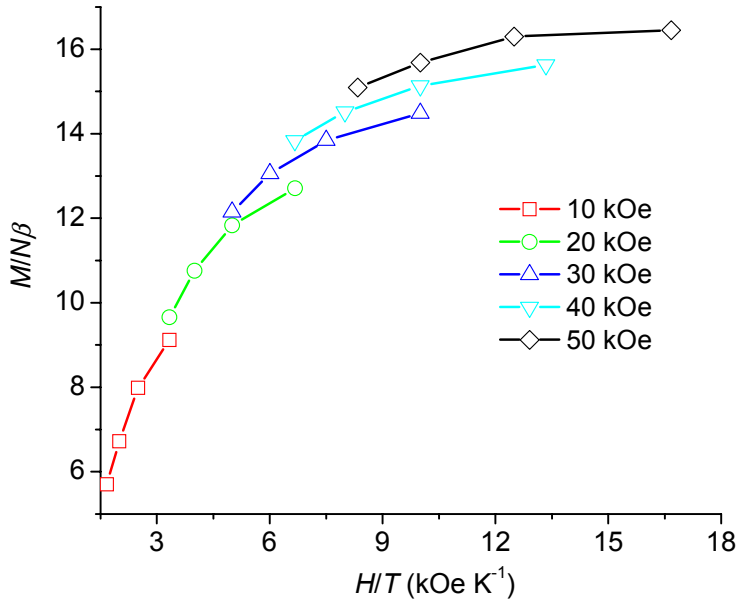

Fig. S7. Magnetization vs. *H*/*T* plot for complex **4**. The lines are guide for the eye.

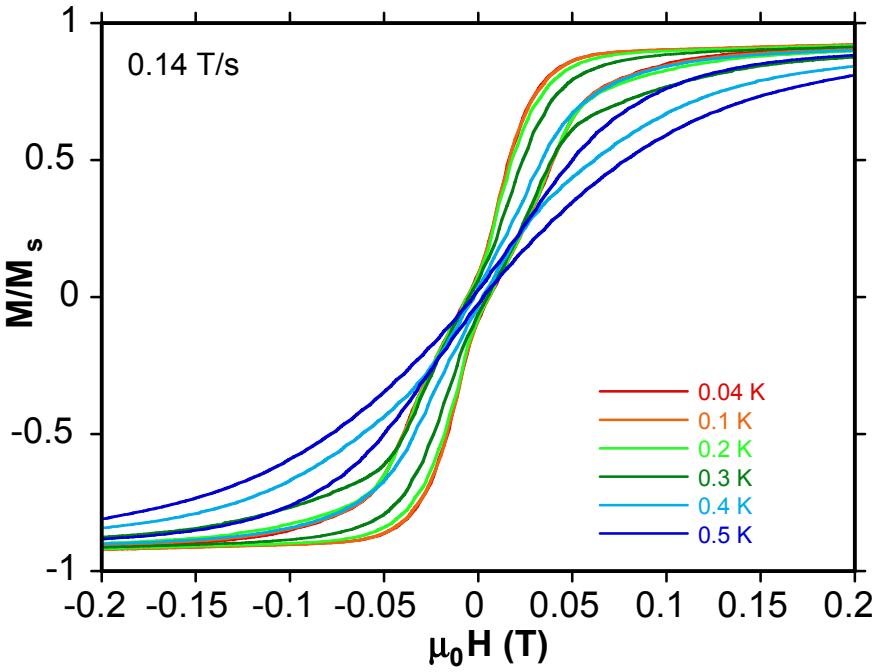

Fig. S8. Hysteresis loop for complex **4** at different temperatures measured at the constant scan magnetic field speed of 0.14 T s^{-1}.