Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information

Encapsulation of a Guest Sodium Cation by Iron(III) tris-(Hydroxamate)s

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Supporting Information

Table S1. Bond distances (Å) and angles (°) for **1**.

Fe1—O1^{i}	1.981 (3)	O2—C1	1.294 (6)
Fe1—O1^{ii}	1.981 (3)	N1—C1	1.283 (6)
Fe1—O1	1.981 (3)	N1—H1	0.8800
Fe1—O2	2.048 (3)	N2—C4	1.328 (7)
Fe1—O2^{ii}	2.048 (3)	N2—C5	1.344 (8)
Fe1—O2^{i}	2.048 (3)	C1—C2	1.477 (7)
Fe1—Na1	3.0414 (12)	C2—C6	1.380 (7)
Na1—O2^{ii}	2.331 (3)	C2—C3	1.394 (7)
Na1—O2^{i}	2.331 (3)	C3—C4	1.382 (8)
Na1—O2	2.331 (3)	C3—H3	0.9500
Na1—O2^{iii}	2.331 (3)	C4—H4	0.9500
Na1—O2^{iv}	2.331 (3)	C5—C6	1.391 (8)
Na1—O2^{v}	2.331 (3)	C5—H5	0.9500
Na1—Fe1^{v}	3.0414 (12)	C6—H6	0.9500
O1—N1	1.396 (6)		
O1^{i}—Fe1—O1^{ii}	94.03 (14)	O2—Na1—Fe1	42.30 (8)
O1^{i}—Fe1—O1	94.02 (14)	O2^{iii}—Na1—Fe1	137.70 (8)
O1^{ii}—Fe1—O1	94.02 (14)	O2^{iv}—Na1—Fe1	137.70 (8)
O1^{i}—Fe1—O2	155.08 (14)	O2^{v}—Na1—Fe1	137.70 (8)
O1^{ii}—Fe1—O2	109.83 (14)	O2^{ii}—Na1—Fe1^{v}	137.70 (8)
O1—Fe1—O2	77.68 (13)	O2^{i}—Na1—Fe1^{v}	137.70 (8)
O1^{i}—Fe1—O2^{ii}	109.83 (14)	O2—Na1—Fe1^{v}	137.70 (8)
O1^{ii}—Fe1—O2^{ii}	77.68 (13)	O2^{iii}—Na1—Fe1^{v}	42.30 (8)
O1—Fe1—O2^{ii}	155.08 (14)	O2^{iv}—Na1—Fe1^{v}	42.30 (8)
O2—Fe1—O2^{ii}	83.09 (14)	O2^{v}—Na1—Fe1^{v}	42.30 (8)
O1^{i}—Fe1—O2^{i}	77.68 (13)	Fe1—Na1—Fe1^{v}	180.0
O1^{ii}—Fe1—O2^{i}	155.08 (14)	N1—O1—Fe1	114.5 (3)
O1—Fe1—O2^{i}	109.83 (14)	C1—O2—Fe1	112.6 (3)

O2—Fe1—O2^{i}	83.09 (14)	C1—O2—Na1	146.6 (3)
O2^{ii}—Fe1—O2^{i}	83.09 (14)	Fe1—O2—Na1	87.72 (11)
O1^{i}—Fe1—Na1	122.36 (11)	C1—N1—O1	114.0 (4)
O1^{ii}—Fe1—Na1	122.36 (11)	C1—N1—H1	123.0
O1—Fe1—Na1	122.36 (11)	O1—N1—H1	123.0
O2—Fe1—Na1	49.98 (9)	C4—N2—C5	117.1 (5)
O2^{ii}—Fe1—Na1	49.98 (9)	N1—C1—O2	121.2 (5)
O2^{i}—Fe1—Na1	49.98 (9)	N1—C1—C2	119.9 (4)
O2^{ii}—Na1—O2^{i}	71.30 (12)	O2—C1—C2	118.9 (4)
O2^{ii}—Na1—O2	71.30 (12)	C6—C2—C3	117.4 (5)
O2^{i}—Na1—O2	71.30 (12)	C6—C2—C1	123.4 (5)
O2^{ii}—Na1—O2^{iii}	108.70 (12)	C3—C2—C1	119.2 (4)
O2^{i}—Na1—O2^{iii}	180.0	C4—C3—C2	119.8 (5)
O2—Na1—O2^{iii}	108.70 (12)	C4—C3—H3	120.1
O2^{ii}—Na1—O2^{iv}	180.0	C2—C3—H3	120.1
O2^{i}—Na1—O2^{iv}	108.70 (12)	N2—C4—C3	123.2 (5)
O2—Na1—O2^{iv}	108.70 (12)	N2—C4—H4	118.4
O2^{iii}—Na1—O2^{iv}	71.29 (12)	C3—C4—H4	118.4
O2^{ii}—Na1—O2^{v}	108.70 (12)	N2—C5—C6	123.4 (5)
O2^{i}—Na1—O2^{v}	108.70 (12)	N2—C5—H5	118.3
O2—Na1—O2^{v}	180.0	C6—C5—H5	118.3
O2^{iii}—Na1—O2^{v}	71.30 (12)	C2—C6—C5	119.2 (5)
O2^{iv}—Na1—O2^{v}	71.30 (12)	C2—C6—H6	120.4
O2^{ii}—Na1—Fe1	42.30 (8)	C5—C6—H6	120.4
O2^{i}—Na1—Fe1	42.30 (8)		

Symmetry codes: (i) *y*, *z*, *x*; (ii) *z*, *x*, *y*; (iii) −*y*, −*z*, −*x*; (iv) −*z*, −*x*, −*y*; (v) −*x*, −*y*, −*z*.

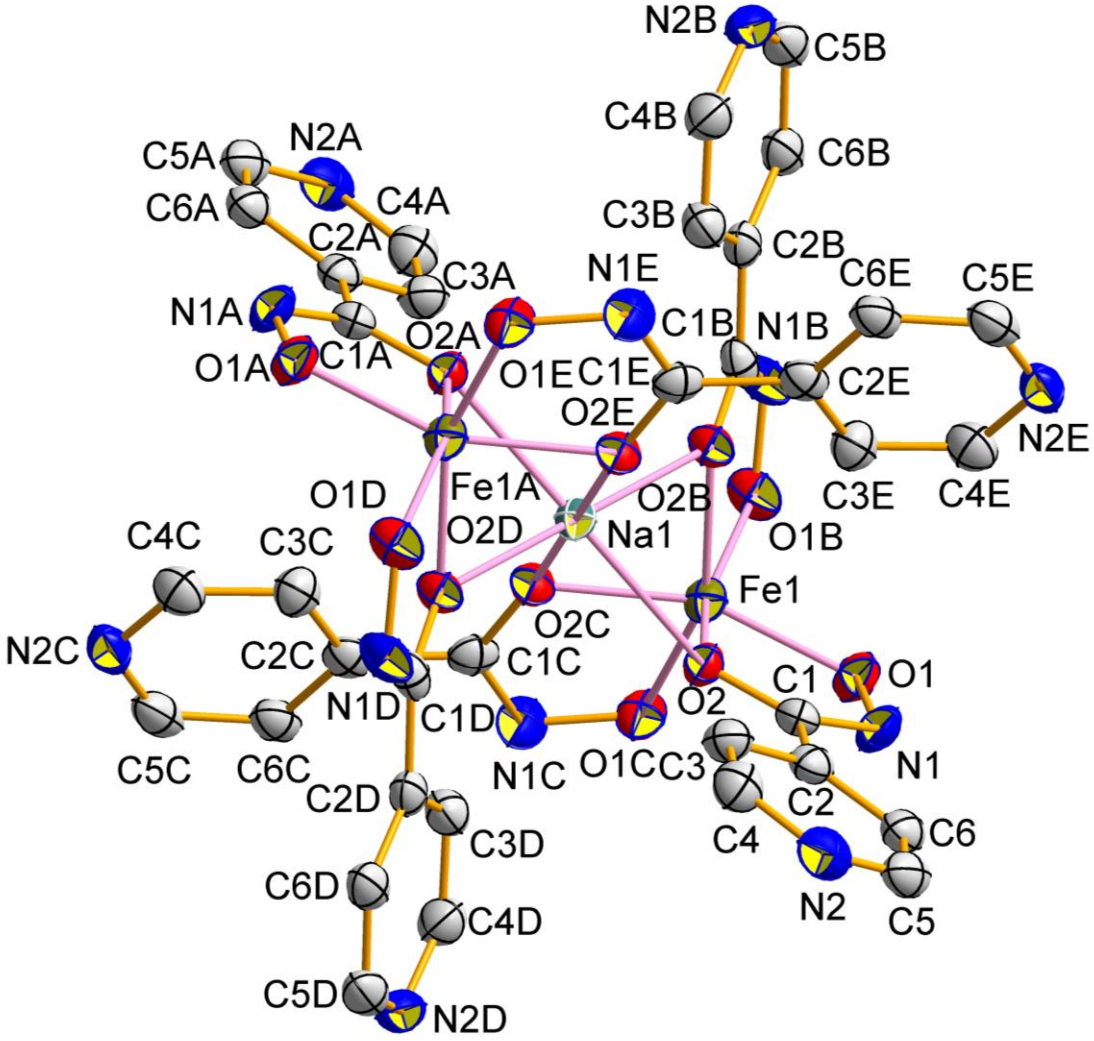

Figure S1. Molecular structure of complex cation in **1** with full numbering scheme. Hydrogen atoms are omitted for clarity. Symmetry codes: (A): -x, -y, -z; (B): y, z, x; (C): z, x, y; (D): -y, -z, -x; (E): -z, -x, -y.

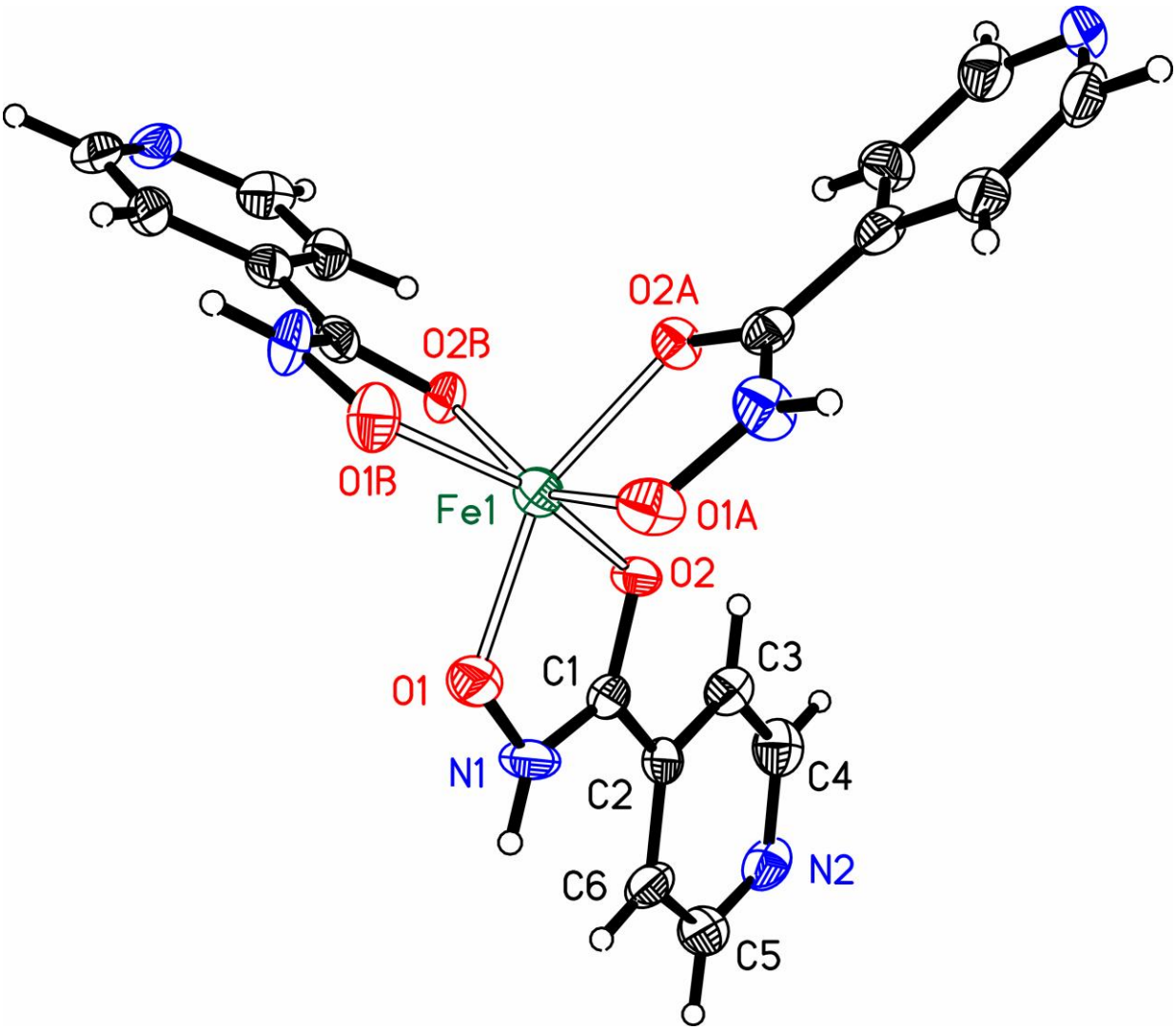

Figure S2. Structure of mononuclear iron(III) tris(hydroxamate) fragment in **1**. Symmetry codes: (A): z, x, y; (B): y, z, x.

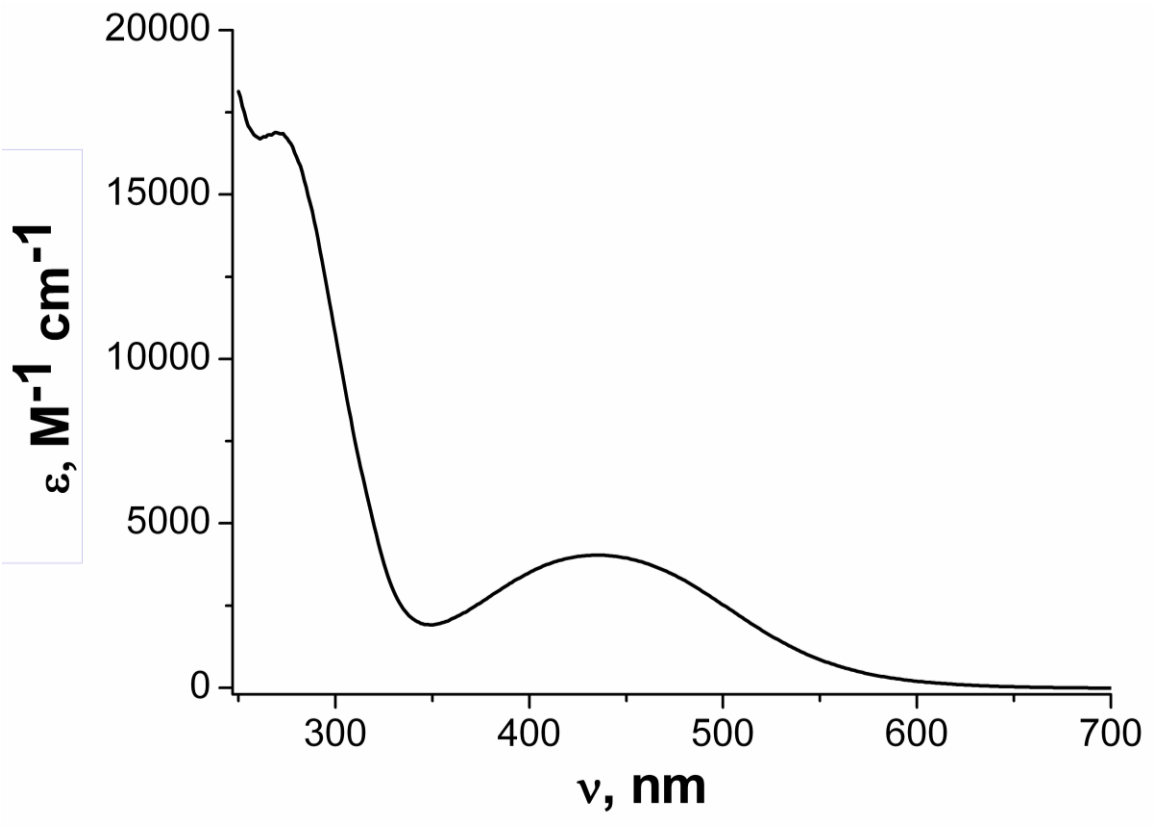

Figure S3. Electronic spectrum of **1** in methanol.

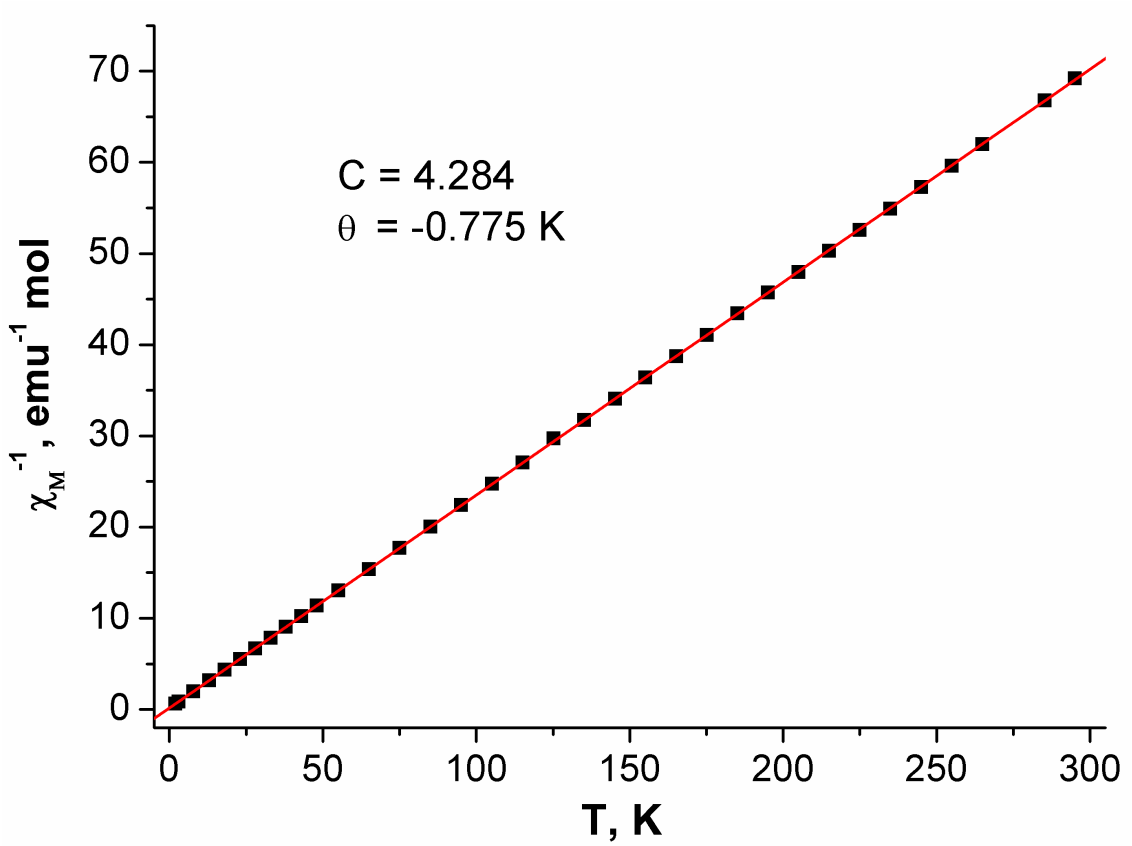

Figure S4. The temperature dependence of the reciprocal molar magnetic susceptibility (χ^{-1}) for **1**. Full red line corresponds to the fit by the Curie-Weiss law.

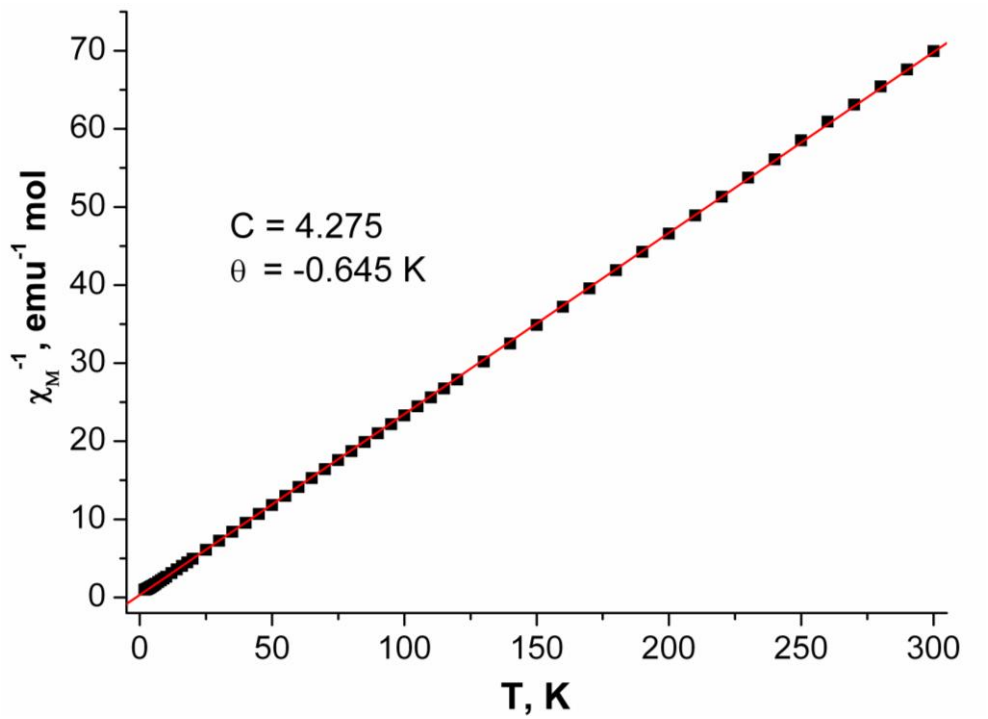

Figure S5. The temperature dependence of the reciprocal molar magnetic susceptibility (χ^{-1}) for $[Fe(4\text{-}PyMHA)_3]\cdot 5.5H_2O$ [4]. Full red line corresponds to the fit by the Curie-Weiss law.