

Electronic Supplementary Information

Self-Assembled Octanuclear Complex Bearing the Uncommon Close-Packed $\{\text{Fe}_4\text{Mn}_4(\mu_4\text{-O})_4(\mu\text{-O})_4\}$ Molecular Core

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Table S1. Selected geometrical parameters (distances/Å and angles/°) for **1**

Fe1–O2	1.933(5)	Mn3–O5	2.256(5)
Fe1–O5	1.964(4)	Mn3–O6	1.920(5)
Fe1–O11	2.026(4)	Mn3–O7	1.873(5)
Fe1–O12	1.975(4)	Mn3–O9	2.197(6)
Fe1–O12 ^a	2.202(4)	Mn3–O12	1.871(4)
Fe1–N3	2.143(6)	Mn3–N4	2.071(6)
Fe2–O3	1.949(5)	Mn4–O1	1.874(5)
Fe2–O8	1.921(5)	Mn4–O3	2.279(5)
Fe2–O11	2.265(5)	Mn4–O4	1.905(5)
Fe2–O11 ^a	1.959(4)	Mn4–O10	2.167(7)
Fe2–O12	2.026(5)	Mn4–O11	1.865(4)
Fe2–N2	2.157(6)	Mn4–N1	2.079(6)
O2–Fe1–O5	99.7(2)	O5–Mn3–O7	95.5(2)
O2–Fe1–O11	89.3(2)	O5–Mn3–O9	169.5(2)
O2–Fe1–O12	161.4(2)	O5–Mn3–O12	77.4(2)
O2–Fe1–O12 ^a	107.0(2)	O5–Mn3–N4	88.5(2)
O2–Fe1–N3	90.2(2)	O6–Mn3–O5 ^a	94.3(2)
O5–Fe1–O11	114.5(2)	O6–Mn3–O9 ^a	91.8(2)
O5–Fe1–O12	76.9(2)	O6–Mn3–N4 ^a	176.4(2)
O5–Fe1–O12 ^a	149.2(2)	O7–Mn3–O6 ^a	92.6(2)
O5–Fe1–N3	83.8(2)	O7–Mn3–O9	92.8(2)
O11–Fe1–O12	75.9(2)	O7–Mn3–O12	172.6(2)
O11–Fe1–N3	161.5(2)	O7–Mn3–N4	89.5(2)
O12–Fe1–O11 ^a	81.3(2)	O9–Mn3–O12	94.0(2)
O12–Fe1–O12 ^a	82.2(2)	O9–Mn3–N4	85.1(2)
O12–Fe1–N3	107.4(2)	O12–Mn3–O6 ^a	89.9(2)
O12–Fe1–N3 ^a	81.2(2)	O12–Mn3–N4	88.4(2)
O3–Fe2–O8	99.2(2)	O1–Mn4–O3 ^a	95.3(2)
O3–Fe2–O11	149.6(2)	O1–Mn4–O4	93.8(2)
O3–Fe2–O11 ^a	76.4(2)	O1–Mn4–O10	94.5(2)
O3–Fe2–O12	113.2(2)	O1–Mn4–O11	172.4(2)
O3–Fe2–N2	84.3(2)	O1–Mn4–N1	89.4(2)
O8–Fe2–O11	107.6(2)	O4–Mn4–O3 ^a	96.3(2)
O8–Fe2–O11 ^a	159.9(2)	O4–Mn4–O10	93.7(2)
O8–Fe2–O12	89.7(2)	O4–Mn4–O11	89.8(2)
O8–Fe2–N2	91.2(2)	O4–Mn4–N1	175.9(2)
O11–Fe2–O11 ^a	82.8(2)	O10–Mn4–O3 ^a	165.5(2)
O11–Fe2–O12	81.6(2)	O10–Mn4–O11	92.0(2)
O11–Fe2–N2	81.1(2)	O10–Mn4–N1	83.6(2)
O12–Fe2–O11 ^a	74.6(2)	O11–Mn4–O3 ^a	77.6(2)
O12–Fe2–N2	162.1(2)	O11–Mn4–N1	87.3(2)
N2–Fe2–O11 ^a	107.6(2)	N1–Mn4–O3 ^a	85.9(2)

Symmetry transformations used to generate equivalent atoms: ^a 1–x, y, 1.5–z.