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Supplementary Materials

Tetranuclear Hetro-Metal [$Mn^{III}_2Ni^{II}_2$] Complexes Involving Defective Double-Cubane Structure: Synthesis, Crystal Structures, and Magnetic Properties

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Table S1. Crystal data of **1** and **2**.

Complex	1	2
Empirical Formula	$C_{80}H_{66}Cl_8Mn_2N_4Ni_2O_{14}$	$C_{75}H_{58}Cl_6Mn_2N_6Ni_2O_{14}$
Formula Weight	1818.32	1707.31
Crystal System	monoclinic	triclinic
Space Group	$P2_1/c$ (#14)	$P\bar{1}$ (#2)
a/Å	13.139(4)	11.589(8)
b/Å	10.915(5)	17.362(12)
c/Å	30.879(13)	18.540(11)
α/°	90	98.1991(10)
β/°	102.02(3)	92.4517(10)
γ/°	90	105.645(10)
V/Å^3	4332(3)	3543(4)
Z	2	2
D_{calc}/gcm^{-3}	1.394	1.600
F(000)	1856.00	1740.00
μ(MoKα)/mm^{-1}	1.019	1.169
Radiation	MoKα (λ = 0.71069 Å)	MoKα (λ = 0.71075 Å)
2θmax/°	40.0	54.9
Data/Restraints/Parameters	3969/4/488	14953/0/946
R, R_w	0.0661, 0.2318	0.0977, 0.2531
$(\Delta\rho)_{max}/(\Delta\rho)_{min}$ e$^-$/Å^3	0.88/−0.49	1.25/−0.93
Goodness of Fit Indicator	1.028	1.043
$(\Delta\sigma)_{max}$	<0.001	<0.001
CCDC number	1886404	1886403

Table S2. Bond angles in the coordination spheres of **1**, **2A,** and **2B**.

Bond/Angle	**1** (Å)/(°)	**2A** (Å)/(°)	**2B** (Å)/(°)
O1–Mn1–O2	173.3(3)	177.7(3)	177.3(3)
O1–Mn1–O3	87.2(3)	86.6(2)	85.9(2)
O1–Mn1–O4*	76.2(2)	77.9(2)	78.1(2)
O1–Mn1–O5	90.5(3)	87.0(2)	86.8(2)
O1–Mn1–N1	89.8(3)	89.9(2)	89.2(3)
O2–Mn1–O3	93.4(3)	94.1(2)	95.1(3)
O2–Mn1–O4*	97.1(3)	99.9(2)	99.5(2)
O2–Mn1–O5	93.4(3)	95.2(2)	95.7(2)
O2–Mn1–N1	89.2(3)	89.4(3)	89.8(3)
O3–Mn1–O4*	86.7(2)	87.7(2)	87.7(2)
O3–Mn1–O5	91.6(3)	89.4(2)	89.2(2)
O3–Mn1–N1	175.1(3)	176.5(2)	175.1(2)
O4*–Mn1–O5	166.7(3)	164.77(18)	164.72(19)
O4*–Mn1–N1	88.8(3)	91.3(3)	91.6(2)
O5–Mn1–N1	92.3(3)	90.8(3)	90.2(3)
O1–Ni1–O1*	80.7(2)	82.0(2)	82.0(2)
O1–Ni1–O3	79.2(3)	80.0(2)	79.7(2)
O1–Ni1–O4	97.5(3)	96.2(2)	96.8(2)
O1–Ni1–O6	89.4(3)	88.6(2)	90.6(2)
O1–Ni1–N2	171.8(3)	173.6(2)	173.1(2)
O1*–Ni1–O3	89.1(2)	90.3(2)	89.9(2)
O1*–Ni1–O4	82.1(3)	83.1(2)	80.7(2)
O1*–Ni1–O6	169.4(3)	169.5(2)	172.2(2)
O1*–Ni1–N2	99.2(3)	98.8(3)	102.6(3)
O3–Ni1–O4	171.0(2)	172.8(2)	170.4(2)
O3–Ni1–O6	93.1(3)	92.7(2)	91.3(2)
O3–Ni1–N2	92.6(3)	93.7(2)	95.1(3)
O4–Ni1–O6	95.2(3)	93.4(2)	97.8(2)
O4–Ni1–N2	90.6(3)	90.1(2)	89.0(3)
O6–Ni1–N2	91.1(3)	91.1(3)	85.0(3)

Symmetry code (*): $-x + 1, -y, -z$ (**1**); $-x + 2, -y, -z + 1$ (**2A**); $-x + 2, -y + 1, -z + 2$ (**2B**).

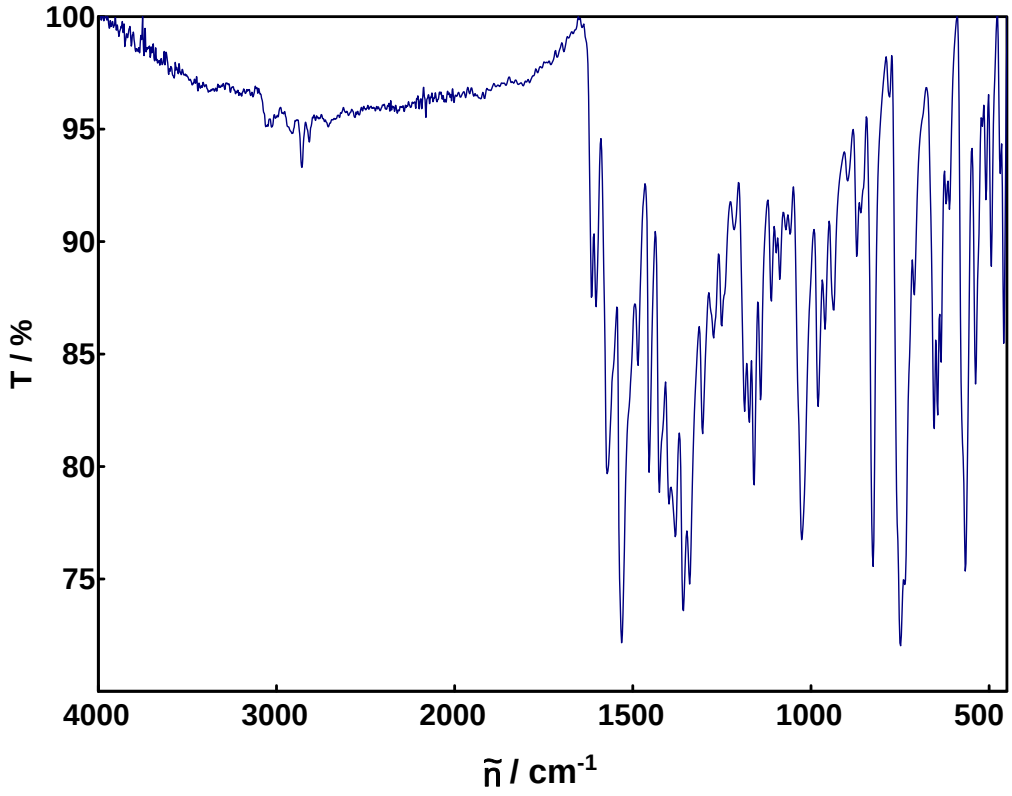

Figure S1. FT-IR spectrum of **1**.

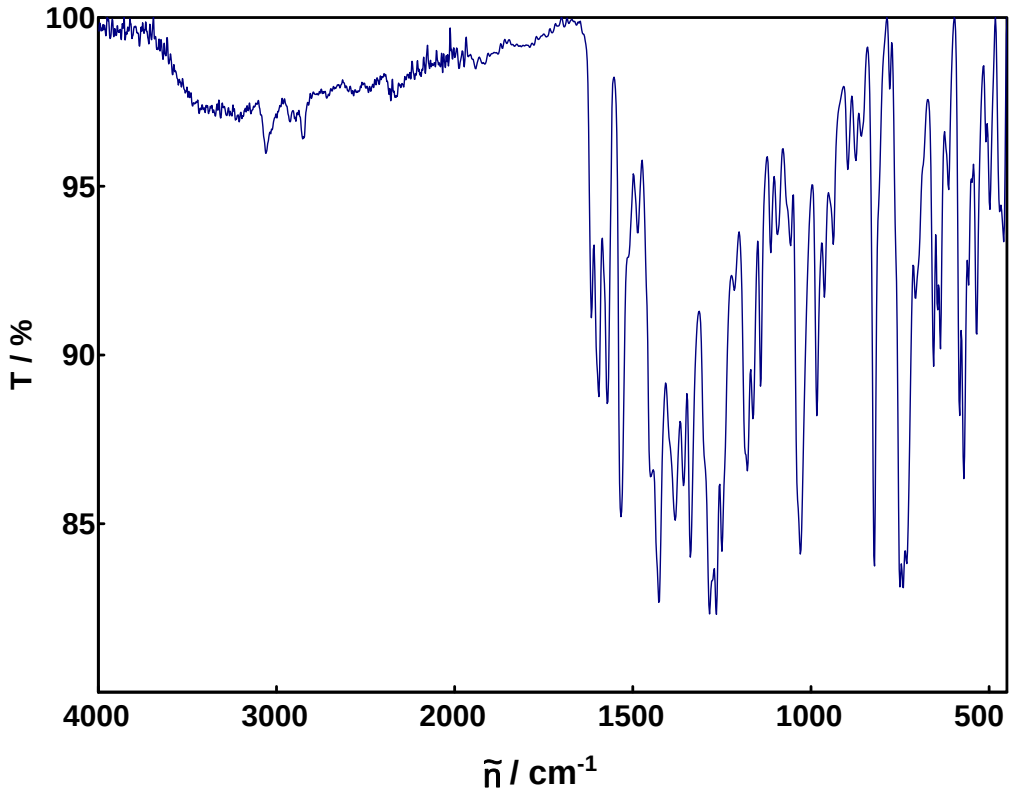

Figure S2. FT-IR spectrum of **2**.

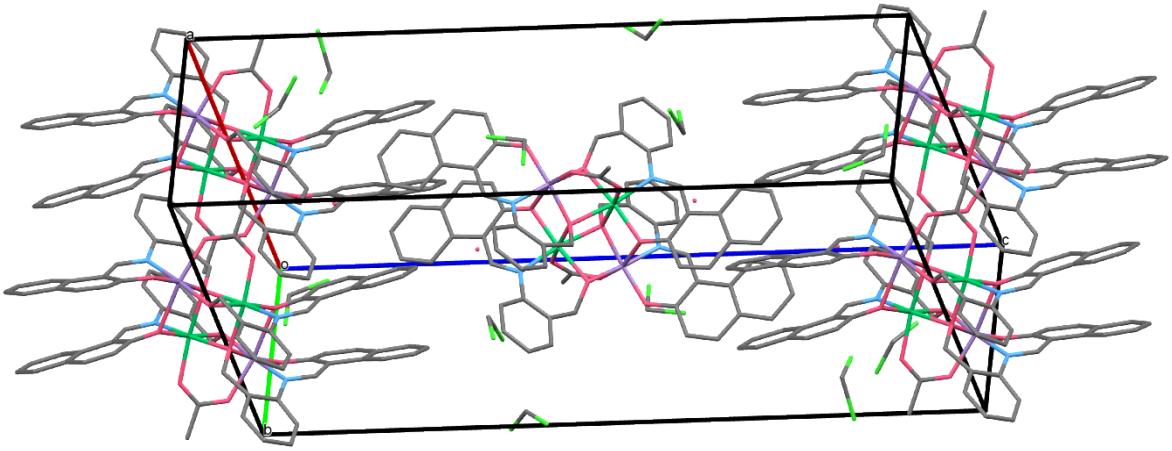

Figure S3. Crystal Packing diagram of **1**.

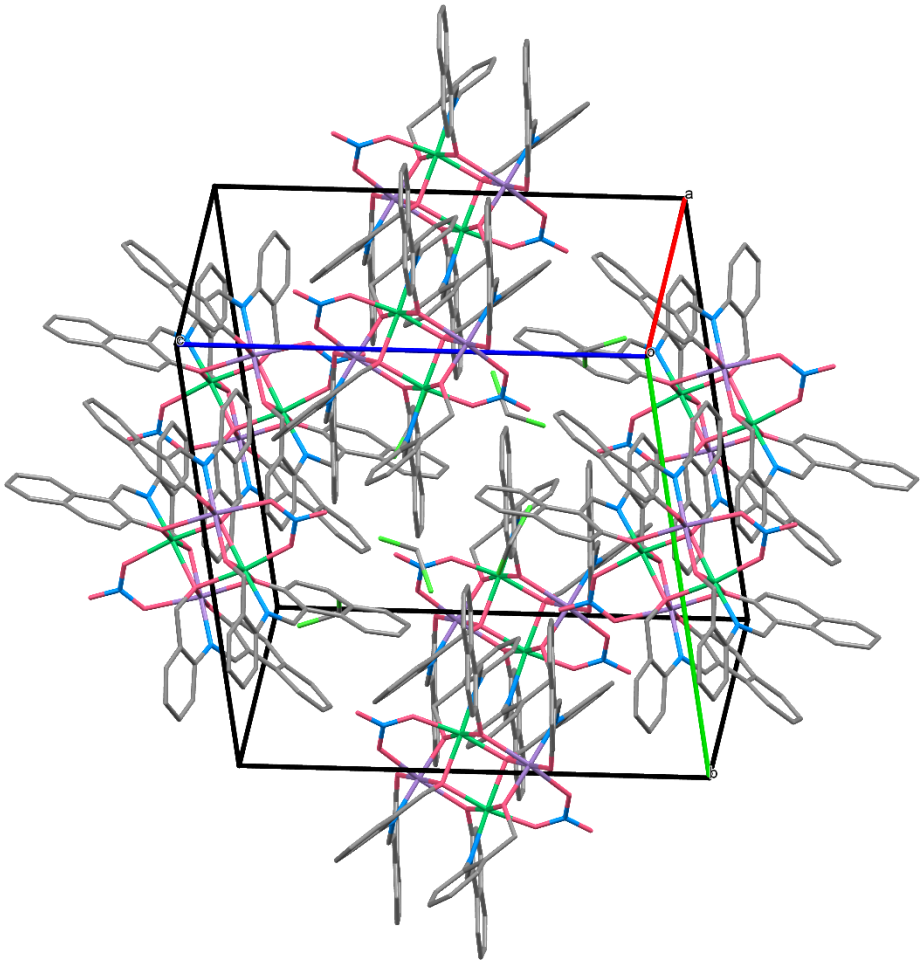

Figure S4. Crystal Packing diagram of **2**.