SUPPLEMENTARY MATERIAL TO

Synthesis, x-ray structure and DFT calculation of magnetic properties of binuclear Ni(II) complex with tridentate hydrazone-based ligand

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ISOLATED YIELDS AND SPECTROSCOPIC DATA OF SYNTHESIZED COMPOUNDS

*(E)-N,N,N-trimethyl-2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)ethan-1-aminium-chloride (**HL**Cl).* Yield 1.17 g (87%). White solid. IR (ATR, cm^{-1}): 3387w, 3127m, 3090m, 3049m, 3016m, 2950s, 1700vs, 1612w, 1549s, 1485m, 1400m, 1300w, 1253w, 1200s, 1153w, 1135m, 1095w, 1073m, 975w, 944w, 914m, 748w, 683w. Anal. Calcd. for $C_{12}H_{19}ClN_4O$ (*FW*: 270.76): C, 53.23; H, 7.07; N, 20.69 %. Found: C, 53.34; H, 7.38; N, 20.49 %. ^{1}H NMR: 11.41 (N-H, s), 4.92 (C10-H_2, s), 3.35 (C11-H_9, s), 2.37 (C8-H_3, s), 8.62 (C3-H, m), 7.45 (C4-H, m), 7.91 (C5-H, td, J^3 = 10 Hz, J^4 = 5 Hz), 8.12 (C6-H, d, J^3 = 10 Hz). ^{13}C NMR: 63.2 (C10), 53.7 (C11), 13.9 (C8), 149.2 (C3), 124.9 (C4), 137.2 (C5), 120.8 (C6), 154.9 (C7), 155.3 (C2), 167.1 (C9).

*$[Ni_2$**L**$_2(\mu$-$_{1,1}$-$N_3)_2(N_3)_2]\cdot 6H_2O$ complex (**1**).* Yield 126 mg (73 %). IR (ATR, cm^{-1}): 3344s, 3036w, 2039vs, 1619w, 1595w, 1540s, 1469m, 1441m, 1399w, 1335w, 1300m,

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1247w, 1200w, 1145w, 1074w, 1026w, 973w, 909w, 781w, 750w, 676w, 571w. Anal. Calcd. for $C_{24}H_{48}N_{20}Ni_2O_8$ (*FW*: 862.24): C, 33.43; H, 5.61; N 32.49 %. Found: C, 33.31; H, 5.69; N 32.24.

SUPPORTING INFORMATION FOR X-RAY CRYSTALOGRAPHY

TABLE S1. Crystal data and structure refinement details for **1**.

	1
formula	$C_{24}H_{48}N_{20}Ni_2O_8$
Fw (g mol^{-1})	862.24
crystal size (mm)	0.20 × 0.20 × 0.05
crystal color	yellow
crystal system	triclinic
space group	*P* –1
a (Å)	8.9538(7)
b (Å)	9.0014(6)
c (Å)	13.1769(11)
α (º)	76.170(6)
β (º)	73.159(7)
γ (º)	82.598(6)
V (Å^3)	984.97(14)
Z	1
calcd density (g cm^{-3})	1.454
F(000)	452
no. of collected reflns	9259
no. of independent reflns	5142
R_{int}	0.0420
no. of reflns observed	4217
no. parameters	266
$R[I > 2\sigma(I)]^a$	0.0495
wR_2 (all data)^b	0.1314
Goof , S^c	1.039
maximum/minimum residual electron density (e Å^{-3})	+1.65/–0.65

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

TABLE S2. Hydrogen-bond parameters for complex **1**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symm. operation on A
O1W–H1W···N3	0.86(5)	2.13(5)	2.982(4)	171(4)	
O2W–H3W···N5	0.84(4)	2.04(4)	2.885(4)	177(5)	
O2W–H4W···O3W	0.84(5)	1.97(5)	2.726(5)	150(5)	
O3W–H5W···N7	0.85(4)	2.18(4)	2.992(5)	160(5)	x, 1+y, z
O3W–H6W···O1W	0.86(4)	1.96(4)	2.748(5)	153(6)	1+x, y, z
Intra C1–H1···O1	0.95	2.55	3.288(3)	135	1-x, -y, 1-z

C2–H2···N10	0.95	2.57	3.451(5)	155	2-x,-y,1-z
C11···H11A···N10	0.98	2.61	3.517(5)	154	-1+x, y, z
Intra C11–H11B···O1	0.98	2.39	2.989(4)	119	
C12–H12C···N7	0.98	2.52	3.429(4)	154	1-x,-y,-z

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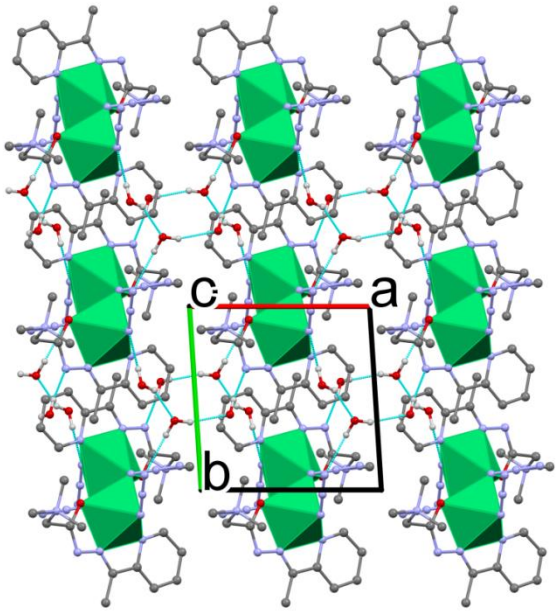

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44 a)

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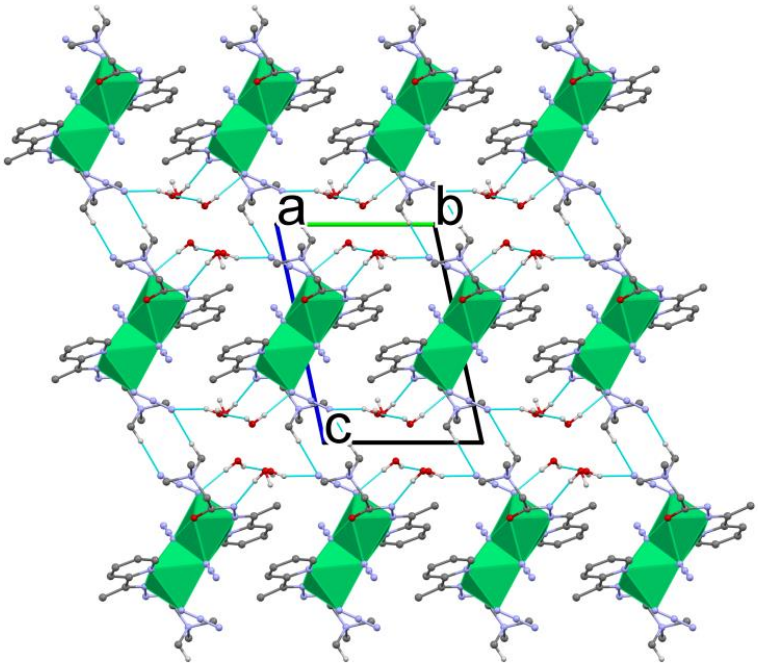
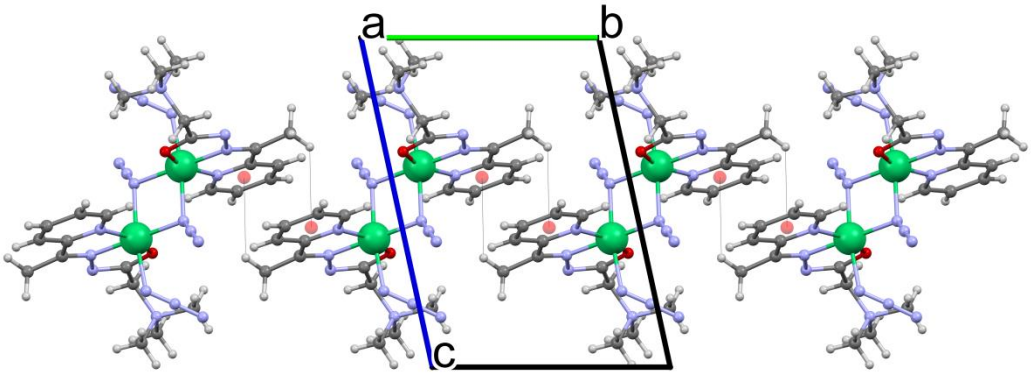


46

47 b)

48



c)

Fig S1. Crystal packing of **1** showing a) 2D layer parallel with the (001) lattice plain generated by intermolecular hydrogen bonding. b) Side view of the layers parallel with the (001) lattice plane showing channels propagating parallel with *a* axis filled with solvent water molecules. Hydrogen atoms have been omitted for the sake of clarity, except those involved in hydrogen bonding. c) C7–H7B···π(py) intermolecular contact connecting dimers of **1** along [010] direction.