Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. 85 (10) S473–S475 (2020) *Supplementary material*

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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J. Serb. Chem. Soc. 85 (10) (2020) 1279–1290

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}): 3387*w*, 3127*m*, 3090*m*, 3049*m*, 3016*m*, 2950*s*, 1700*vs*, 1612*w*, 1549*s*, 1485*m*, 1400*m*, 1300*w*, 1253*w*, 1200*s*, 1153*w*, 1135*m*, 1095*w*, 1073*m*, 975*w*, 944*w*, 914*m*, 748*w*, 683*w*. 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 (δ / ppm): 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 (δ / ppm): 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**$_2$(μ-$_{1,1}$-N_3)$_2$(N_3)$_2$]·6H_2O complex (**1**).* Yield 126 mg (73 %). IR (ATR, cm^{-1}): 3344*s*, 3036*w*, 2039*vs*, 1619*w*, 1595*w*, 1540*s*, 1469*m*, 1441*m*, 1399*w*, 1335*w*, 1300*m*, 1247*w*, 1200*w*, 1145*w*, 1074*w*, 1026*w*, 973*w*, 909*w*, 781*w*, 750*w*, 676*w*, 571*w*. 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.

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SUPPORTING INFORMATION FOR X-RAY CRYSTALOGRAPHY

TABLE S-I. Crystal data and structure refinement details for **1**

	1
Empirical 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)
Volume, Å^3	984.97(14)
Z	1
Calculated density, g cm^{-3}	1.454
F(000)	452
Reflections collected	9259
Independent reflections	5142
R_{int}	0.0420
Reflections observed	4217
Parameters	266
Final *R* indices [$I > 2\sigma(I)$][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 S-II. Hydrogen-bond parameters for complex **1**

D–H···A	Distance, Å			Angle, °	Symm.
	D–H	H···A	D···A	D–H···A	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

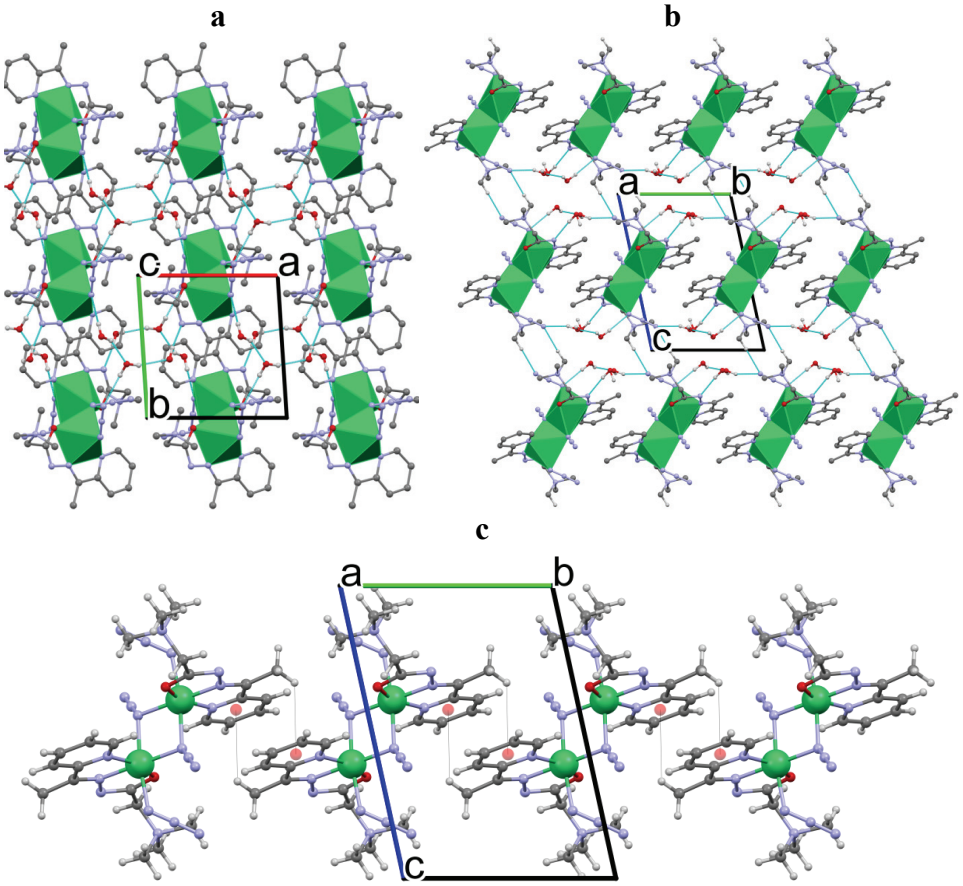

Fig S-1. Crystal packing of **1** showing: a) 2D layer parallel with the (001) lattice plain generated by intermolecular hydrogen bonding. b) Side view of the layers parallel with the (001) lattice plane showing channels propagating parallel with *a* axis filled with solvent water molecules. Hydrogen 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.