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Synthesis, crystal structure, magnetic properties and DFT study of dinuclear Ni(II) complex with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent

Mima Č. Romanović[a], Božidar R. Čobeljić[a], Andrej Pevec[b], Iztok Turel[b], Vojislav Spasojević[c], Arshak A. Tsaturyan[d], Igor N. Shcherbakov[d], Katarina K. Anđelković[a], Marina Milenković[e], Dušanka Radanović[f], Milica R. Milenković[a*]

[a]*Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia*

[b]*Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia*

[c]*Institute of Nuclear Sciences 'Vinča', Condensed Matter Physics Laboratory, P.O. Box 522, 11001 Belgrade, Serbia*

[d]*Department of Chemistry, Southern Federal University, Zorge St. 7, 344090, Rostov-on-Don, Russia*

[e]*Faculty of Pharmacy, Department of Microbiology and Immunology, University of Belgrade, Vojvode Stepe 450, 11221 Belgrade, Serbia*

[f]*Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, P.O. Box 815, 11000 Belgrade, Serbia*

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* Corresponding author: Milica R. Milenković, e-mail: mrm@chem.bg.ac.rs

Table S.4. Total energies (*E*, a.u.), relative energies (*ΔE*, given in kcal mol^{-1}) and expectation values of the spin-squared ($<S^2>$) operator calculated for HS and BS states in the high-spin and broken symmetry (BS) states of the complex **1** calculated by the DFT method with different functionals

Table S.5. Selected optimized structural parameters in HS and BS spin states, obtained with various DFT functionals

Table S.6. Mulliken spin populations (ρ) and total charges (q) on atoms of the exchange fragment (B3LYP*/6-311G(d,p)) in high (HS) and low spin states (BS)

Figure S.1. Perspective view of the crystal structure of **1** showing infinite chains based on N(amide)···O(solvent water)···N(azido end-on) intermolecular hydrogen bonds. The neighboring chains are linked through π···π and C–H···π(ring) interactions. By reason of clarity, methanol and a series of hydrogen atoms are omitted.

Table S.1. Intra- and intermolecular π···π interaction parameters for $[Ni_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]\cdot H_2O\cdot CH_3OH$ complex

Cg(I)[a]	Cg(J)[a]	Cg(I) –Cg(J)[b] (Å)	α[c] (°)	β[d] (°)	γ[e] (°)	Sym. code on (J)
Intramolecular						
Cg(A'')	Cg(B'')	3.588(2)	9.8(1)	17.0	13.8	*x*, *y*, *z*
Cg(A'')	Cg(B')	4.557(2)	8.0(1)	47.1	41.1	*x*, *y*, *z*
Cg(A')	Cg(B'')	4.787(2)	10.8(1)	46.1	42.8	*x*, *y*, *z*
Intermolecular						
Cg(A')	Cg(A')	4.172(2)	0.0	35.4	35.4	-*x*, 2-*y*, -*z*
Cg(A'')	Cg(A')	4.512(2)	2.7(1)	40.0	42.2	-*x*, 2-*y*, -*z*

[a] Labels of aromatic rings: (A') = N1A, C8A′,C4A′,C2A-C4A; (A'') = C4A′,C8A′,C5A-C8A; (B') = N1B,C4B′,C8B′,C2B-C4B; (B'') = C4B′,C8B′,C5B-C8B.
[b] Cg(I) –Cg(J) = Distance between ring centroids (Ang.).
[c] α = Dihedral angle between planes (I) and (J) (Deg).
[d] β = Angle between Cg(I)–Cg(J) vector and normal to plane (I) (Deg).
[e] γ = Angle between Cg(I) –Cg(J) vector and normal to plane (J) (Deg).

Table S.2. Intermolecular C–H···π(quinoline) interaction parameters for $[Ni_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]\cdot H_2O\cdot CH_3OH$ complex

C–H	Cg(J)	H···Cg (Å)	H···(quinoline J)[a] (Å)	C–H···Cg (°)	γ [b] (°)	Sym. code on (J)
C7A–H7A	Cg(B")	2.95	-2.88	128	12.4	*-x*, 1/2+*y*, 1/2-*z*

[a] Perpendicular distance of H to ring plane (J) (Ang.).

[b] γ = Angle between H···Cg line and perpendicular H···(ring plane) line (Deg).

Table S.3. Hydrogen bond parameters (Å,°) for $[Ni_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]\cdot H_2O\cdot CH_3OH$ complex

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Sym. code on A
O1SA–H1SA ···N6ZA	0.97(9)	2.1(1)	2.80(2)	126(7)	
O1SA–H2SA ···N3B	1.00(5)	1.98(6)	2.917(9)	155(7)	*x*, 3/2-*y*, -1/2+*z*
O1SB–H1SB···N6ZB	0.99(9)	2.15(11)	3.048(13)	151(9)	

Table S.4. Total energies (*E*, a.u.), relative energies (*ΔE*, given in kcal mol^{-1}) and expectation values of the spin-squared ($<S^2>$) operator calculated for HS and BS states in the high-spin and broken symmetry (BS) states of the complex **1** calculated by the DFT method with different functionals

Functional	Spin state	*S*	*E*, a.u.	Δ*E*, kcal/mol	S^2
B3LYP	HS	2	-5427.396931		6.020
	BS	0	-5427.396188	0.47	2.015
B3LYP*	HS	2	-5405.442710		6.020
	BS	0	-5405.442149	0.35	2.016
PBE0	HS	2	-5424.064214		6.022
	BS	0	-5424.063412	0.50	2.016
TPSSh	HS	2	-5427.496460		6.023
	BS	0	-5427.495768	0.43	2.019

Table S.5. Selected optimized structural parameters in HS and BS spin states, obtained with various DFT functionals

Functional	Spin state	Ni1A–N4Z	N4Z–Ni1B	Ni1B–N1Z	N1Z–Ni1A	Ni1A–N4Z–Ni1B	Ni1A–N1Z–Ni1B
B3LYP*	HS	2.2458	2.0915	2.1424	2.0901	98.8	102.3
	BS	2.2551	2.0925	2.1476	2.0945	98.9	102.4
B3LYP	HS	2.1457	2.0613	2.0984	2.1058	99.7	99.8
	BS	2.1520	2.0644	2.1033	2.1093	99.7	99.9
PBE0	HS	2.1084	2.0384	2.0832	2.0895	99.5	98.7
	BS	2.1129	2.0409	2.0873	2.0933	99.5	98.7
TPSSh	HS	2.1760	2.0558	2.1043	2.0554	99.1	101.5
	BS	2.1829	2.0585	2.1090	2.0588	99.1	101.6
Experimental data XRD		2.1400(19)	2.0819(18)	2.1339(18)	2.0851(17)	102.01(8)	102.11(7)

Table S.6. Mulliken spin populations (ρ) and total charges (q) on atoms of the exchange fragment (B3LYP*/6-311G(d,p)) in high (HS) and low spin states (BS)

Functional	Spin state	Spin density Ni1A/atomic charge	Spin density Ni1B/atomic charge	Spin density N1Z/atomic charge	Spin density N4Z/atomic charge
B3LYP*	HS	1.629/1.36	1.653/1.372	0.025/-0.764	0.015/-0.726
	LS	1.633/1.361	-1.656/1.372	-0.012/-0.764	0.000/-0.725
B3LYP	HS	1.673/1.38	1.700/1.402	0.026/-0.801	0.022/-0.781
	LS	1.678/1.381	-1.705/1.403	-0.014/-0.802	-0.003/-0.782
PBE0	HS	1.708/1.426	1.733/1.451	0.015/-0.850	0.015/-0.833
	LS	1.714/1.427	-1.739/1.452	-0.011/-0.851	-0.002/-0.834
TPSSh	HS	1.617/1.409	1.640/1.416	0.019/-0.821	0.011/-0.794
	LS	1.622/1.409	-1.644/1.416	-0.011/-0.822	0.001/-0.795

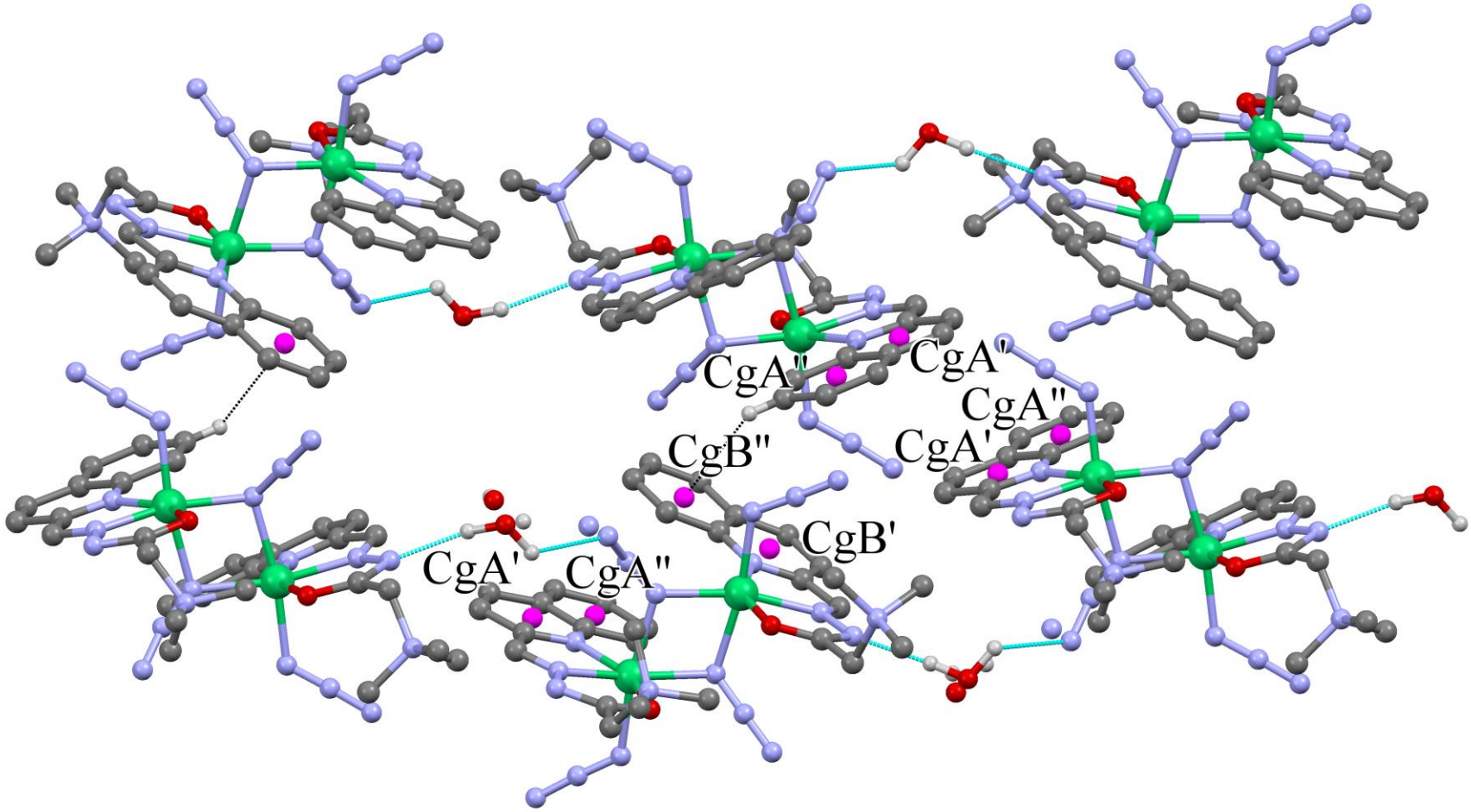

Figure S.1. Perspective view of the crystal structure of **1** showing infinite chains based on N(amide)···O(solvent water)···N(azido end-on) intermolecular hydrogen bonds. The neighboring chains are linked through π···π and C–H···π(ring) interactions. By reason of clarity, methanol and a series of hydrogen atoms are omitted.