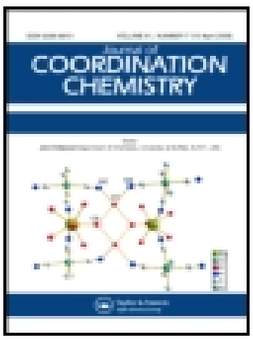

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Nickel versus copper: Enhanced antibacterial activity in a series of new nickel(II) Schiff base complexes

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Five new Ni(II) Schiff base complexes $[NiL^x(Solv)_2]$ denoted by NiL^x, x = 1-5, were synthesized and characterized. The Schiff base ligands were synthesized from the condensation of 5-bromo-2-hydroxy-3-nitrobenzaldehyde with different aliphatic and aromatic diamines. The X-ray crystal structure of NiL^3 was determined. The ligands and complexes were tested as antibacterial agents against two Gram(+) and two Gram(-) human pathogenic bacteria. The complexes showed moderate antibacterial activity against both Gram type bacteria. The new Ni(II) complexes showed enhanced antibacterial activity compared to the previously reported Cu(II) complexes of the same ligands.

Keywords: Schiff base; Antibacterial; Nickel(II) complexes

1. Introduction

There has been interest in study of the biological applications of coordination compounds [1-3]. The ligand and the metal center cooperatively create a chance for the synthesis of new metallo-drugs. Indeed, fine tuning of the electronic properties of the central metal ion is possible with the possibility of introducing different substituents with electron withdrawing and/or electron donating features on the ligands. Steric factors are also tunable with those substituents, which is important in some drug-target interactions. The metal center can also modify both the extent and direction of the pharmacological properties of the ligand [4, 5]. A variety of Schiff base ligands and their metal complexes have been prepared and studied for their catalytic properties, metal

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bio-sites modeling, biological properties, *etc.* [6-10]. Among them, tetradentate N_2O_2 Schiff base ligands are perhaps the most widely studied ones.

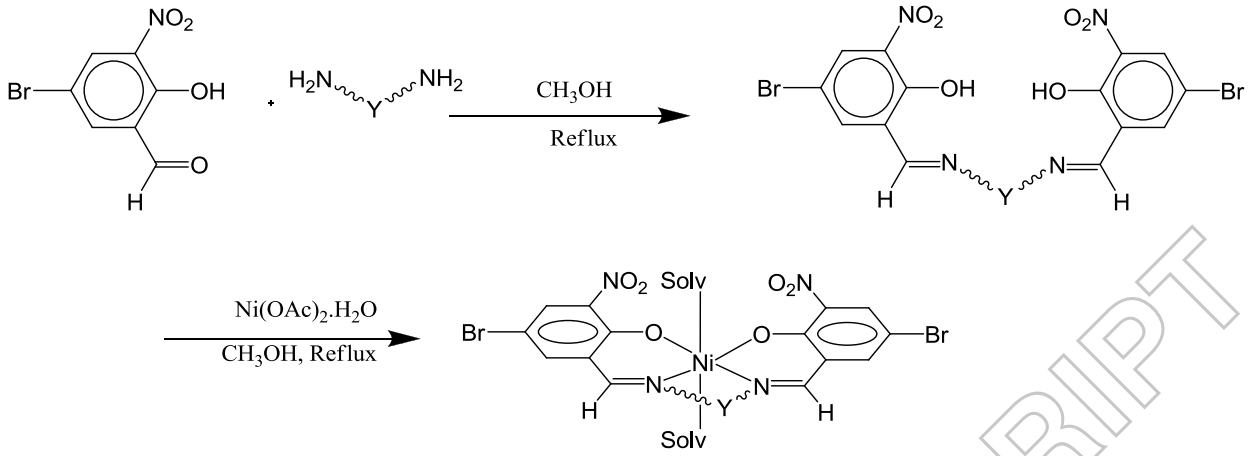
Nickel is an essential trace element in living systems. Examples include the active site of at least nine enzymes such as urease and carbon monoxide dehydrogenase [11, 12]. The quest for understanding the modes of action of nickel in living systems is an active area of research. Nickel(II) Schiff base complexes have been studied for their biological properties [13-17]. Apart from the biological importance of nickel Schiff base complexes, these complexes have also been studied for their catalytic [18-20] and magnetic [21-23] properties. In continuation of our previous studies, we report herein the synthesis, characterization and antibacterial properties of five new Ni(II) Schiff base complexes. Our previous studies as well as the study of other researchers [13, 14] have shown that the presence of more electronegative substituents on the Schiff base ligand increases the antibacterial activity. Therefore, we deliberately designed a series of Schiff base ligands derived from condensation of different diamines with 5-bromo-3-nitro-2-hydroxybenzaldehyde. Nickel(II) complexes of these ligands were prepared and characterized. Crystal structure of one complex was determined. The complexes have general formula $[NiL^x(Solv)_2]$ in which L represents the dianionic Schiff base ligand and Solv represents the solvent molecules axially coordinated to nickel. Antibacterial activities of these complexes were investigated against four human pathogenic bacteria, *Escherichia coli* (Gram negative), *Salmonella typhi* (Gram negative), *Staphylococcus aureus* (Gram positive) and *Bacillus subtilis* (Gram positive). These Ni(II) complexes showed higher antibacterial activity against the studied bacteria than previously reported Cu(II) complexes of the same ligands [13].

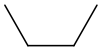
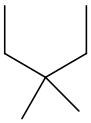
2. Experimental

2.1. *Materials and methods*

All chemicals and solvents were purchased from Merck chemical company, Germany, and were used as received. 5-Bromo-2-hydroxy-3-nitrobenzaldehyde was synthesized as described [24]. The ligands were synthesized following literature procedure [25-27]. Melting points were obtained on a thermoscientific 9100 apparatus. Elemental analyses were performed on a Perkin-Elmer 2400II CHNS-O analyzer. IR spectra were obtained as KBr plates using a Bruker FT-IR instrument. UV-vis spectra were obtained on a Shimadzu UV-1650PC spectrophotometer. X-ray diffraction measurements for NiL^3 were made on a STOE IPDSII diffractometer with graphite

monochromated MoKα radiation. Data were collected at 293(2) K in a series of ω scans in 1° oscillations and integrated using the Stoe X-AREA software package. A numerical absorption correction was applied using PLATON software. The data were corrected for Lorentz and polarization effects. The structure was solved by direct methods using SIR2004. The non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using SHELXL. All the hydrogens were placed at calculated positions and constrained to ride on their parent atoms. Details concerning collection and analysis for NiL^3 are reported in table 1.



Y	Ligand	Complex
	H_2L^1	NiL^1
	H_2L^2	NiL^2
	H_2L^3	NiL^3
	H_2L^4	NiL^4
	H_2L^5	NiL^5

Scheme 1. The procedure of the synthesis of the ligands and complexes.

2.2. *Synthesis of the complexes*

The Ni(II) Schiff base complexes were synthesized by the equimolar reaction of the corresponding Schiff base ligands and nickel(II) acetate in methanol. The obtained precipitates were then recrystallized in DMSO to yield pure crystals of the target complexes. The NiL^x complexes were obtained with two coordinated DMSO molecules as shown in scheme 1 except for NiL^3, for which the details are given in results and discussion.

2.2.1. Synthesis of NiL^1. 1 mmol (0.2 g) of H_2L^1 was dissolved in 10 mL methanol and was heated to reflux. To this solution, a methanolic solution of 1 mmol of $Ni(OAc)_2{\cdot}H_2O$ (0.07 g in 10 mL) was added. The reaction mixture was refluxed for 4 h. The orange solid product was collected by filtration, washed with 15 mL of hot methanol and air dried. Recrystallization from DMSO yielded 0.2 g (89%) of the target complex. Selected FT-IR (KBr, cm^{-1}): 1627($\nu_{C=N}$), 1521(ν_{NO2}), 1228(ν_{C-O}). UV-vis in DMSO [λ_{max} nm (ε $M^{-1}cm^{-1}$)]: 268 (187200), 446 (68000), 632 (290). Anal. Calcd. for $C_{20}H_{22}Br_2N_4NiO_8S_2$: C, 32.94; H, 3.02; N, 7.69. Found: C, 32.85; H, 3.11; N, 7.75.

2.2.2. Synthesis of NiL^2. This complex was synthesized following a similar procedure as described for NiL^1 except H_2L^2 was used instead of H_2L^1. Yield was 0.15 g (82.5%). Selected FT-IR (KBr, cm^{-1}): 1629($\nu_{C=N}$), 1531(ν_{NO2}), 1230(ν_{C-O}). UV-vis in DMSO [λ_{max} nm (ε $M^{-1}cm^{-1}$)]: 267 (13200), 427 (9500), 600 (120). Anal. Calcd. for $C_{21}H_{24}Br_2N_4NiO_8S_2$: C, 33.94; H, 3.23; N, 7.54. Found: C, 33.89; H, 3.18; N, 7.60.

2.2.3. Synthesis of NiL^3. This complex was synthesized following a similar procedure as described for NiL^1 except H_2L^3 was used instead of H_2L^1. Yield was 0.15 g (83%). Selected FT-IR (KBr, cm^{-1}): 1639($\nu_{C=N}$), 1528(ν_{NO2}), 1230(ν_{C-O}). UV-vis in DMSO [λ_{max} nm (ε $M^{-1}cm^{-1}$)]: 267 (13100), 425 (7200), 595 (100). Anal. Calcd. for $C_{23}H_{29}Br_2N_4NiO_{8.5}S_2$: C, 35.40; H, 3.72; N, 7.18. Found: C, 35.46; H, 3.68; N, 7.22.

2.2.4. Synthesis of NiL^4. This complex was synthesized following a similar procedure as described for NiL^1 except H_2L^4 was used instead of H_2L^1. Yield was 0.18 g (97%). Selected FT-IR (KBr, cm^{-1}): 1612($\nu_{C=N}$), 1523(ν_{NO2}), 1205(ν_{C-O}). UV-vis in DMSO [λ_{max} nm (ε $M^{-1}cm^{-1}$)]: 266 (33800), 315 (31500), 445 (19000), 750 (80). Anal. Calcd. for $C_{28}H_{22}Br_2N_4NiO_8S_2$: C, 40.75; H, 2.67; N, 6.79. Found: C, 40.68; H, 2.61; N, 6.72.

2.2.5. Synthesis of NiL^5. This complex was synthesized following a similar procedure as described for NiL^1 except H_2L^5 was used instead of H_2L^1. Yield was 0.14 g (80%). Selected FT-IR (KBr, cm^{-1}): 1616($\nu_{C=N}$), 1523(ν_{NO2}), 1213(ν_{C-O}). UV-vis in DMSO [λ_{max} nm (ε $M^{-1}cm^{-1}$)]:

267 (23780), 318 (14760), 445 (16790), 745 (80). Anal. Calcd. for $C_{25}H_{37}Br_2N_4NiO_8S_2$: C, 37.34; H, 4.60; N, 6.97. Found: C, 37.29; H, 4.65; N, 6.92.

2.3. *Antibacterial studies*

2.3.1. Bacterial strains. The metal complexes were tested against *Salmonella typhi* (ATCC 19430, Gram negative), *Escherichia coli* (ATCC 25922, Gram negative), *Staphylococcus aureus* (ATCC 25923, Gram positive) and *Bacillus subtilis* (ATCC No. 6633, Gram positive).

2.3.2. Determination of minimum inhibitory concentration (MIC) and minimal bactericidal concentration (MBC). Minimum inhibitory concentration (MIC, μg mL^{-1}) was determined by the broth micro-dilution method following the procedures recommended by the National Committee for Clinical Laboratory Standards [28, 29]. MICs were defined as the lowest concentrations of compounds which inhibit the growth of microorganisms. All tests were performed in triplicate. Minimal bactericidal concentration (MBC) was also measured following a standard procedure [30]. 100 μL volumes of all clear (no growth) tubes from a dilution MIC test was spread onto separate agar plates and incubated at 37 °C for 24 h. The MBC (μg mL^{-1}) was defined as the lowest concentration of the complex for which no growth occurred.

3. Results and discussion

3.1. *Spectroscopic characterization*

The most significant signal in the IR spectrum of a Schiff base ligand or complex is the stretching vibration of the imine group (C=N). This signal usually shifts to lower wavenumbers upon coordination of the iminic nitrogen to a transition metal ion. In the IR spectra of the ligands, the presence of an intense band at ~1640 cm^{-1} was previously assigned to the stretching vibration of the azomethine (C=N) groups. In the IR spectra of these Ni(II) complexes, these signals shifted to lower wavenumbers indicating the incorporation of the nitrogens of the C=N groups in coordination.

In the UV-vis spectra of the ligands with aliphatic diamines, two intense bands were observed at 270 nm and 480 nm which were assigned to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, respectively. In the UV-vis spectra of the ligands with aromatic diamines, the afore-mentioned bands were also observed and a new band appeared at 330 nm. These new bands were assigned

to the π→π* transitions mainly concentrated on the phenyl rings of the diamine moiety. In the UV-vis spectra of the complexes, the bands assigned to the π→π* transitions appeared at almost the same wavelengths while the bands assigned to the n→π* transitions in the ligands were absent and instead; new bands were observed at wavelengths around 430 nm which were assigned to the MLCT transitions [26, 31]. The signals due to the d-d transitions in octahedral Ni(II) Schiff base complexes are usually observed at 400-500 nm ($^3A_{2g}\rightarrow{}^3T_{1g}(P)$) and 600-800 nm ($^3A_{2g}\rightarrow{}^3T_{1g}(F)$). A third signal at above 900 nm ($^3A_{2g}\rightarrow{}^3T_{2g}(F)$) is sometimes not observed since it does not fall in the range covered by the commonly used instruments [32]. In our complexes, the first signals were masked by the intense n→π* signal but the weak signals due to the $^3A_{2g}\rightarrow{}^3T_{1g}(F)$ were observed at the expected area.

3.2. *Description of the crystal structure of NiL^3*

Single crystals suitable for X-ray crystallography were obtained from slow evaporation from NiL^3 solution in DMSO in about one month. Unfortunately, attempts to prepare suitable single crystals from other complexes failed. Figure 1 shows the ORTEP representation of the $[NiL^3(DMSO)_2]$ and $[NiL^3(DMSO)(H_2O)]$ complexes. Table 1 collects a summary of the crystallographic data and selected bond lengths and angles are collected in table 2. The unit cell of the NiL^3 complex consists of two chemically unequivalent molecules. In both molecules, the central Ni(II) ion is coordinated to a basal dianionic Schiff base ligand, however, these two molecules differ in the axial coordination. One of the two molecules contains two axial DMSO ligands (figure 2, right (**A**)), while in the other one (figure 2, left (**B**)) the axial positions are occupied by one DMSO and one H_2O ligand. All the Ni-O and Ni-N bond distances are normal and are similar to previously reported octahedral Ni(II) complexes. The axial O-Ni-O angle is 176.1(2)° in (**A**) and 178.91(19)° in (**B**) which show slight deviations from the ideal octahedron. The equatorial O-Ni-O and N-Ni-N angles also deviate from ideal octahedral in both (**A**) and (**B**), and hence, the geometry around Ni(II) is considered as slightly distorted octahedron (table 2). Other bond lengths and angles around the central metal ions collected in table 2 confirm the distorted octahedral geometry. O7 and O8 of one of the NO_2 groups in (**A**) are disordered and are shown as O7A, O7 B, O8A and O8B in the ORTEP drawing (figure 1). One uncoordinated DMSO is also present in the unit cell which is not shown in the ORTEP drawing for clarity. The six-membered chelate ring in the current Schiff base ligand is comprised of a

1,3-diamino-2,2-dimethylpropane fragment (neopentandiamine). The conformation of the six-membered chelate ring in both structures is very clearly a chair somewhat flattened at the N3-Ni-N4 site as taken from the structure of [$NiL^3(DMSO)_2$] and at the N7-Ni-N8 site as taken from [$NiL^3(DMSO)(H_2O)$] (figure 2) [33]. The dihedral angles between the planes defined by the two phenyl rings of the salicylaldehyde moieties in (**A**) and (**B**) are 51.79(2)° and 67.10(2)°, respectively. The six-membered rings in the diamine moieties have distorted chair structure.

3.3. *Antibacterial studies*

The presence of more electronegative substituents on the Schiff base ligands increases the antibacterial activity of ligands and their metal complexes [13, 14]. To further explore this idea, we have synthesized a salicylaldehyde derivative with two electronegative substituents, *i.e.* bromo and nitro substituents at the 5- and 3-position of the salicylaldehyde. Copper(II) complexes of these ligands were previously synthesized and their antibacterial effect was studied [13]. In this work, the synthesis of a series of the corresponding Ni(II) complexes is being reported. The synthesized Ni(II) complexes were screened for their *in vitro* antibacterial activity against two Gram positive *(S. aureus* and *B. subtilis*) and two Gram negative (*E. coli* and *S. typhi*) human pathogenic bacteria according to literature protocols [28-30]. The results of the antibacterial studies of the NiL^x complexes as well as kanamycin as the standard drug are collected in table 3. The Ni(II) complexes showed remarkable antibacterial activity against studied bacteria. Comparison of these data with those of the Cu(II) analogues revealed that the Ni(II) complexes showed increased antibacterial activity [13]. For example, the [CuL^2] complex in the reported work, which was the most active antibacterial agent, had MIC values 525, 375, 325 and 450 μg mL^{-1}, respectively, for *E. coli*, *S. typhi*, *S. aureus* and *B. subtilis*. The corresponding Ni(II) complex (NiL^3) showed values of 175, 125, 75 and 75 μg mL^{-1} for the same bacteria, indicating involvement of the central metal in the antibacterial properties of transition metal complexes. These complexes are octahedrally surrounded by the ligands, while the corresponding copper(II) complexes were square planar. By increasing the number of substituents (*i.e.* the presence of two axial ligands) the lipophilicity of the complexes could be increased and, hence, the antibacterial properties of the complexes increased [31, 34]. The ligands [13] and $Ni(OAc)_2$ did not show activity, which confirms that complexation is important in the observed antibacterial activity. Complexes with aliphatic diamines were more active than

the aromatic analogues, which suggest contribution of the ligands and supports the idea of cooperation of the ligands and central metals in such biological activities.

4. Conclusion

Five new Ni(II) Schiff base complexes were synthesized and characterized by various spectroscopic and analytical methods. The X-ray crystal structure of NiL^3 was obtained. The new complexes were screened for potential antibacterial activity against four human pathogenic bacteria. Comparison with the results of the previously reported copper(II) complexes showed that, by changing from Cu(II) to Ni(II), the antibacterial properties of these complexes was considerably improved.

References

[1] C.O. Rodriguez de Barbarin, N.A. Bailey, D.E. Fenton, Q. He. *J. Chem. Soc., Dalton Trans.*, 161 (1997).

[2] S. Ren, R. Wang, K. Komatsu, P. Bonaz-Krause, Y. Zyrianov, C.E. McKenna, C. Csipke, Z.A. Tokes, E.J. Lien. *J. Med. Chem.*, **45**, 410 (2001).

[3] N. Raman, A. Kulandaisamy, C. Thangaraja, K. Jeyasubramanian. *Transition Met. Chem.*, **28**, 29 (2003).

[4] M.T.H Tarafder, T. Khoo, K.A. Crouse, A.M. Ali, B.M. Yamin, H. Fun. *Polyhedron*, **21**, 2691 (2002).

[5] R.C. Elder, E.A. Blubaugh, W.R. Heineman, P.J. Burke, D.R. McMillin. *Inorg. Chem.*, **22**, 2777 (1983).

[6] R.C. Maurya, B.A. Malik, J.M. Mir, P.K. Vishwakarma, D.K. Rajak, N. Jain. *J. Coord. Chem.*, **68**, 2902 (2015).

[7] I.P. Ejidike, P.A. Ajibade. *J. Coord. Chem.*, **68**, 2552 (2015).

[8] D. Pucci, A. Bellusci, A. Crispini, M. Ghedini, M. La Deda. *Inorg. Chim. Acta*, **357**, 495 (2004).

[9] M. Amirnasr, R. Sadeghi Erami, K. Mereiter, K. Schenk Joß, S. Meghdadi, S. Abbasi. *J. Coord. Chem.*, **68**, 616 (2015).

[10] C. Biswas, M.G.B. Drew, A. Figuerola, S. Gómez-Coca, E. Ruiz, V. Tangoulis, A. Ghosh. *Inorg. Chim. Acta*, **363**, 846 (2010).

[11] S.B. Mulrooney, R.P. Hausinger. *FEMS Microbiol. Rev.*, **27**, 239 (2003).

[12] H. Bian, J. Wang, Y. Wei, J. Tang, F. Huang, D. Yao, Q. Yu, H. Liang. *Polyhedron*, **90**, 147 (2015).

[13] N. Imani, M. Behzad, H. Amiri Rudbari, G. Bruno, H. Samari Jahromi, A. Khaleghian. *J. Coord. Chem.*, **68**, 2296 (2015).

[14] M. Layek, M. Ghosh, M. Fleck, R. Saha, D. Bandyopadhyay. *J. Coord. Chem.*, **67**, 3371 (2014).

[15] D. Sakthilatha, R. Rajavel. *J. Chem. Pharm. Res.*, **5**, 57 (2013).

[16] R. Pagadala, P. Ali, J.S. Meshram. *J. Coord. Chem.*, **62**, 4009 (2009).

[17] C.J. Dhanaraj, J. Johnson. *J. Coord. Chem.*, **68**, 2449 (2015).

[18] M. Kalita, P. Gogoi, P. Barman, B. Sarma, A.K. Buragohain, R.D. Kalita. *Polyhedron*, **74**, 93 (2014).

[19] P.Gogoi, S. Hazarika, M.J. Sarma, K. Sarma, P. Barman. *Tetrahedron*, **70**, 7484 (2014).

[20] A. Golcu, M. Tumer, H. Demirelli, R.A. Wheatley. *Inorg. Chim. Acta*, **358**, 1785 (2005).

[21] T. Akitsu, Y. Einaga. *Polyhedron*, **24**, 1869 (2005).

[22] K. Nakajima, Y. Ando, H. Mano, M. Kojima. *Inorg. Chim. Acta*, **274**, 184 (1998).

[23] M.F. Cain, S.C. Reynolds, B.J. Anderson, D.S. Glueck, J.A. Golen, C.E. Moore, A.L. Rheingold. *Inorg. Chim. Acta*, **369**, 55 (2011).

[24] A.B.E.. Lovett, E. Roberts. *J. Chem. Soc.*, 1975 (1928).

[25] Z. Abbasi, M. Behzad, A. Ghaffari, H.A. Rudbari, G. Bruno. *Inorg. Chim. Acta*, **414**, 78 (2014).

[26] M. Pooyan, A. Ghaffari, M. Behzad, H. Amiri Rudbari, G. Bruno. *J. Coord. Chem.*, **66**, 4255 (2013).

[27] D.M. Boghaei, A. Bezaatpour, M. Behzad. *J. Coord. Chem.*, **60**, 973 (2007).

[28] Clinical and Laboratory Standards Institute, *Performance Standards for Antimicrobial Susceptibility Testing: Nineteenth Informational Supplement M100–S19*, Clinical and Laboratory Standards Institute, Wayne, PA (2009).

[29] E. Goldman, L.H. Green, *Practical Handbook of Microbiology*, 2nd Edn., (2009) 37–39, CRC Press, Taylor & Francis Group, New York.

[30] A.W. Bauer, W.M. Kirby, J.C. Sheris, M. Turck. *Am. J. Clin. Pathol.*, **45**, 493 (1966).

[31] P.V. Kumar, P. Radhakrishnan. *Inorg. Chim. Acta*, **375**, 84 (2011).

[32] Z. Afrasiabi, E. Sinn, W. Lin, Y. Ma, C. Campana, S. Padhye. *J. Inorg. Biochem.*, **99**, 1526 (2005).

[33] M. Damercheli, D. Dayyani, M. Behzad, B. Mehravi, M. Shafiee Ardestani. *J. Coord. Chem.*, **68**, 1500 (2015).

[34] N. Dharamaraj, P. Viswanathamurthi, K. Natarajan. *Transition Met. Chem.*, **26**, 105 (2001).

Table 1. Crystallographic data for NiL^3.

Formula	$C_{46}H_{58}Br_4N_8Ni_2O_{17}S_4$
Formula weight	1560.26
Crystal system	Monoclinic
Space group	P21/ c
T (K)	293
λ (Å)	0.71073
Unit cell dimensions	
a (Å)	12.073(2)
b (Å)	10.848(2)
c (Å)	48.674( ) ***[au: the esd is missing]***
α (°)	90
β (°)	102.13(3)
γ (°)	90
Volume ($Å^3$)	6232(2)
Z	4
μ (mm^{-1})	3.37
Radiation type	Mo *K*α
Crystal description	Block
Crystal color	Dark-orange
Crystal size (mm)	0.18 × 0.12 × 0.10
Calculated density (g cm^{-3})	1.663
Absorption coefficient (mm^{-1})	3.372
F(000)	3144
θ range for data collection (°)	1.9 to 25
Limiting indices	-14≤ h ≤ 14
	-12≤ k ≤ 12
	-57≤ l ≤ 57
Data / restraints / parameters	10812 / 23 / 753
Total reflections	31293
Unique reflections (R_{int})	10812 (R_{int} = 0.120)
Completeness	98.4% (θ = 25.00)
Refinement method	MULTI-SCAN
Goodness-of-fit on F^2	1.067
Final R index [I > 2σ(I)]	R_1 = 0.0880, wR_2 = 0.1664
R index [all data]	R_1 = 0.1511, wR_2 = 0.1975
Largest difference peak and hole (e $Å^3$)	0.688 and -0.724

Table 2. Selected bond lengths (Å) and angles (°) in the two chemically unequivalent molecules of NiL^3.

$[NiL^3(DMSO)_2]$		$[NiL^3(DMSO)(H_2O)]$	
Bond lengths (Å)		Bond lengths (Å)	
Ni1—O6	2.007(5)	Ni2—O11	2.062(5)
Ni1—O3	2.023(5)	Ni2—O13	2.069(4)
Ni1—O4	2.109(5)	Ni2—O16	2.025(5)
Ni1—O5	2.111(5)	Ni2—O12	2.116(5)
Ni1—N4	2.042(6)	Ni2—N7	2.029(6)
Ni1—N3	2.055(6)	Ni2—N8	2.036(6)
Bond angles (°)		Bond angles (°)	
O6—Ni1—O3	87.96(19)	O16—Ni2—N7	91.9(2)
O6—Ni1—N4	173.8(2)	O16—Ni2—N8	90.4(2)
O3—Ni1—N4	88.1(2)	N7—Ni2—N8	93.0(2)
O6—Ni1—N3	88.6(2)	O16—Ni2—O11	90.35(19)
O3—Ni1—N3	175.6(2)	N7—Ni2—O11	177.5(2)
N4—Ni1—N3	95.5(2)	N8—Ni2—O11	88.2(2)
O6—Ni1—O4	92.8(2)	O16—Ni2—O13	89.27(19)
O3—Ni1—O4	89.3(2)	N8—Ni2—O13	179.7(2)
N3—Ni1—O4	88.1(2)	O11—Ni2—O13	91.95(18)
O6—Ni1—O5	90.8(2)	O16—Ni2—O12	178.91(19)
O3—Ni1—O5	89.1(2)	N7—Ni2—O12	88.5(2)
N4—Ni1—O5	84.3(2)	N8—Ni2—O12	90.6(2)
N3—Ni1—O5	93.7(2)	O11—Ni2—O12	89.28(19)
O4—Ni1—O5	176.1(2)	O13—Ni2—O12	89.72(19)

Table 3. MIC and MBC values for the Ni(II) complexes against the studied bacteria (μg mL^{-1}).

	NiL^1		NiL^2		NiL^3		NiL^4		NiL^5		Kanamycin	
	MIC	MBC	MIC	MBC	MIC	MBC	MIC	MBC	MIC	MBC	MIC	MBC
E. coli	100	125	225	225	175	175	250	275	275	475	4	3.8
S. typhi	75	125	175	225	125	150	225	225	225	275	3.3	3.2
S. aureus	100	125	100	100	75	100	325	350	325	325	3.2	3
B. subtilis	150	175	225	225	75	125	525	525	375	475	4	3.6

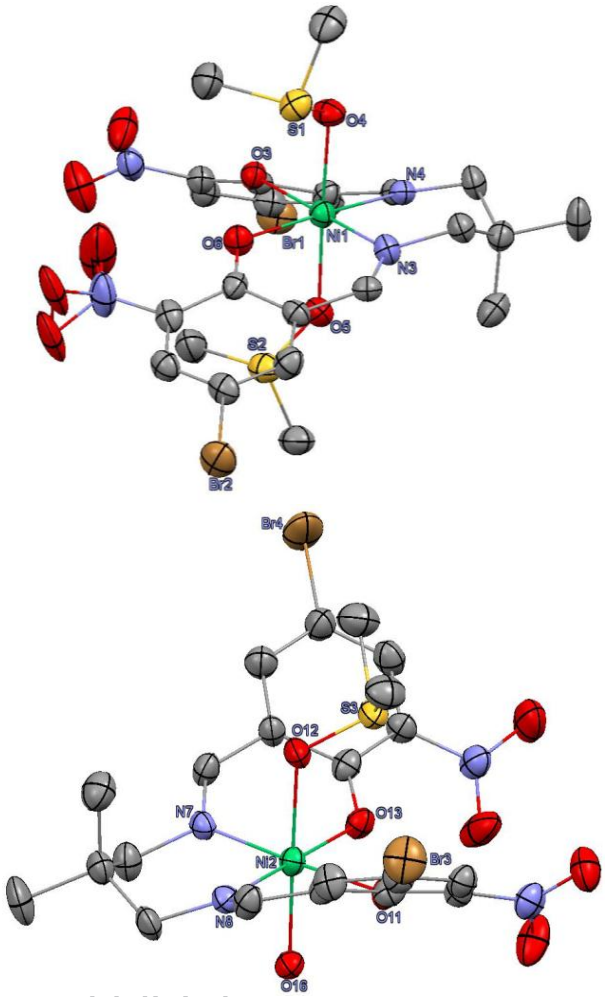


Figure 1. ORTEP representation of the two related molecules in the unit cell of NiL^3, $[NiL^3(DMSO)_2]$ (left) and $[NiL^3(DMSO)(H_2O)]$ (right). Displacement ellipsoids are drawn at the 50% probability level. Uncoordinated and disordered solvent of crystallization (DMSO) and hydrogens are omitted for clarity.

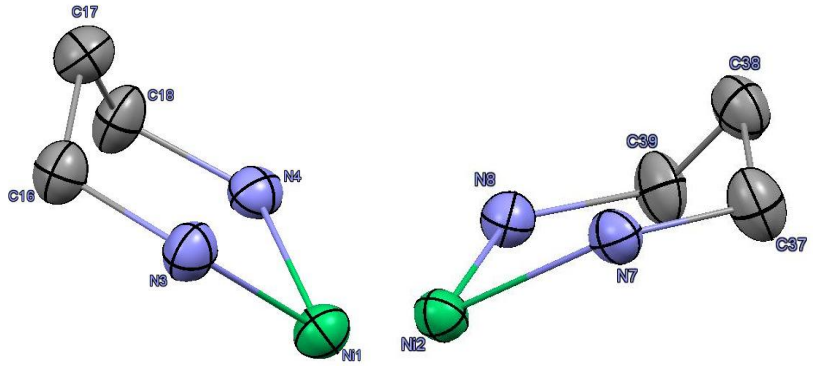


Figure 2. The conformation of the six-membered chelate ring (neopentandiamine fragment) in $[NiL^3(DMSO)_2]$ (left) and $[NiL^3(DMSO)(H_2O)]$ (right).

Graphical abstract