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Synthesis and XRD of neutral NiL complex using unsymmetrical ONNO tetradentate schiff base: Hirschfeld, spectral, DFT and thermal analysis

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ABSTRACT

The unsymmetrical tetradentate ONNO Schiff base 6,6'-((1E,1'E)-((2-methylpropane-1,2-diyl)bis(azanylylidene))bis(methanylylidene))bis(2,4-di-tert-butylphenol) (H₂L) was prepared following a slightly modified known condensation reaction. The neutral NiL complex has been synthesized in high yield via [1H₂L:1Ni(II)] direct addition. The XRD-measurement reflects a Ni^{II} center with slightly distorted square planar geometry. Moreover, the lattice is stabilized by a number of H-bond and $H \dots \pi$ stacking interactions. The structure connections have been illustrated by electrostatic potential surface (Molecular Electrostatic Potential, MEP) and Hirschfeld surface (HSA) and Fingerprint (FP) analysis to support such interactions. IR and UV-visible spectra were measured to compare free H₂L with NiL behaviors. The DFT-optimized structure was compared to the XRD-structure parameters. NiL reflects high thermal stability and decomposed mainly via one-step to form NiO as the final product.

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1. Introduction

There is a huge number of reports on Schiff bases (S.Bs) and their transition metal complexes including tetradentate S.Bs with ONNO type of ligands [1–5]. This is because S.B metal complexes are becoming increasingly important as antimicrobial agents and involved in the biochemical basis for the role of extensive effects of metals, e.g. zinc in cell division [6–12]. A motivating fact about S.Bs is that they can be easily obtained under mild reaction conditions and in high percentage yield [12–20]. Also, they are successful models of biological systems and they have unique properties, e.g. the azomethine linkage which is responsible for medical actions: e.g. the delivery of doxorubicin from biodegradable PEG hydrogels can form Schiff base linkages [14–22]. Noticeably, more symmetrical ONNO types, when compared to

unsymmetrically substituted S.Bs, are known, although unsymmetrically substituted S.Bs as polymerization catalysts are found to be more effective than symmetrically substituted S.B metal complexes [23, 24]. Related examples of nickel complexes have been reported recently [25–27]. Given these facts, we have been stimulated to study the unsymmetrical (H_2L : *N,N'*-bis(3,5-di-t-butylsalicylidene)-1,2-diamino-2-methylpropane) ligand and its nickel complex **NiL**. Interestingly, H_2L possesses four tertiary butyl groups at two different positions on each ring; hence, it enhances solubility in many organic solvents [13]. In addition, H_2L favors monomeric complexes due to the steric hindrance on the ligand. In this study, the steric effect from bulky groups of this Salen complex has suppressed the formation of oxo dimeric or polymeric metal complexes [28–30].

2. Experimental and methodology

2.1. Chemicals, instruments and computation

Chemicals which were used in this study were received from Sigma-Aldrich. HSA was carried out using Crystal Explorer Version 3.1 software [31]. MS were measured on a Varian MAT 711. CHN: Perkin-Elmer Series I1 Analyzer 2400. IR (ν/cm^{-1}) were recorded on a Nicolet Nexus spectrometer. ¹³C and ¹H NMR were carried out on a JEOL ECS 400 spectrometer. The UV-vis spectrophotometer was measured on a ThermoScientific Genesys 10 s. The salicylaldimine **H**₂L used in this study was obtained through condensation of two equivalents of commercially available 3,5-di-tert-butyl-2-hydroxybenzaldehyde with 2-methylpropane-1,2-diamine according to a standard literature procedure with a slight modification [29]. The DFT-computations were carried out in gaseous phase using Gaussian09 software at the B3LYP/DFT level with the 6-311 G(d,p) basis set for all the light atoms; for Cd and I their potential effective core LANL2DZ was also performed using Gaussian09 software [32].

2.2. Synthesis

[2,2'-{(2-methylpropane-1,2-diyl)bis[(azanylylidene)methanylylidene]}bis(4,6-dit-butylphenolato)]-(oxido)-nickel, NiL. H₂L (0.50 g, 0.96 mmol) and Ni(OAc)₂·2H₂O (0.24 g, 0.96 mmol) were added to a two-necked flask charged with a stir bar under argon gas in the presence of Et₃N (0.26 mL, 0.19 g, 1.92 mmol). A mixture of degassed (degassed with argon for 10 min) methanol and chloroform (30 mL) in 5:1 ratio was added and stirred under reflux overnight. The solvents were reduced to one-third, using a vacuum pump, and placed in an ice bath for 35 min. The mixture was filtered in air and the product then washed well with cold ethanol (20 ml) and ice water (10 mL) kept in the fridge beforehand. The yield was (0.43 g, 78%). HRMS (ESI) m/z calc. (C₃₄H₅₀N₂NiO₂) 576.32, found 576.32 (M-H).

2.3. Xrd data collection

The X-ray data for the **NiL** complex were recorded at 100(2) K on a Bruker APEX-II CCD diffractometer, with 0.71073 Å Mo-Ka radiation. The procedure and data reduction

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Table 1.	Crystal	data	for	NiL.
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Chemical formula	C ₃₄ H ₅₀ N ₂ NiO2
CCDC	1992035
<i>M</i> _r	577.47
Crystal system, space group	Monoclinic, P2 ₁ /c
Temperature (K)	100
a, b, c (Å)	10.0272(7), 27.2922(15), 11.6233(7)
β (°)	90.622(4)
V (Å ³)	3180.7(3)
Z	4
Radiation type	Cu <i>Κ</i> α
$\mu (mm^{-1})$	1.11
Crystal size (mm)	0.07 imes 0.02 imes 0.003
Diffractometer	Bruker APEX-II CCD
No. of measured, independent and	18737, 4282, 3763
observed $[I > 2\sigma(I)]$ reflections	
R _{int}	0.052
θ_{max} (°)	58.8
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.555
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.085, 0.217, 1.08
No. of reflections, parameters	4282, 367
Δho_{max} , Δho_{min} (e Å ⁻³)	0.87, -0.49



Scheme 1. Synthesis of unsymmetrical ligand (H₂L) and its NiL complex.

were obtained using SAINT PLUS [33]. The structure was solved using the SHELXS structure solution program by direct methods and refined with the SHELXL [34, 35] refinement package using least squares minimization. The geometrical calculations were carried out using PLATON [36] and the diagrams were generated using MERCURY [37]. The crystal data are illustrated in Table 1.

3. Results and discussion

3.1. Synthesis and CHN analysis

The desired S.B, H_2L of type ONNO tetradentate ligand, was synthesized following a slightly modified known condensation reaction [29] (see Supporting Information). The reaction of H_2L with Ni(OAc)₂·2H₂O, in 1:1 molar ratio, progressed in a mixture of solvents (degassed methanol and chloroform, 1:5 ratio) in the presence of triethylamine to afford the **NiL** complex in high yield as illustrated in scheme 1. Elemental analysis indicated the theoretical values, for the formation of 1:1 nickel complex, were in agreement with the actual results (Table 2).

The **NiL** complex is stable in air, colored, a non-hygroscopic solid and melts at a higher temperature. The nickel complex is not soluble in water; however, it is soluble in many common organic solvents. The **H₂L** ligand coordinated to the Ni center in a tetradentate mode, using ONNO donor sites of the azomethine-N and phenolic-O (scheme 1).

Table 2. Physical data for compounds H₂L and NiL.

Cpd.	Color	T (°C)	C% (found)	C% (Calc.)	H (found)	H (Calc.)	N (found)	N (Calc.)
H₂L	Yellow	165-167	78.43	78.41	10.07	10.6	5.42	5.35
NiL	Green	>360	70.91	70.72	8.97	8.73	4.88	4.85



Figure 1. NiL complex structural belongings (a) ORTEP, (b) optimized B3LYP structure, (c) H-bonds and (d) $2H \dots C = C$ interactions.

3.2. Nil solid-state XRD and DFT structures

The solid-state ORTEP structure of the desired **NiL** complex is illustrated together with the DFT-optimized structure (Figures 1(a,b)); XRD/DFT selected bond lengths and angles are illustrated in Table 3. The neutral **NiL** complex crystallized in a monoclinic lattice, space group $P_{2_1/c}$, without any solvent molecules in the crystal lattice. The Ni(II) ion was found to be surrounded by 2 N-imine and 2 O-phenolic atoms, where each N atom is *trans* to an O atom to form three new five-membered rings via metal center coordination, which have also been observed by DFT structural optimization. A slightly distorted square–planar geometry around Ni(II) with t ~ $-15.55(^{\circ})$ was observed by both DFT and XRD. The bond lengths of Ni–N were found to be ~1.84 and Ni–O ~ 1.83 Å; the main angles around the center are N(1)–Ni–N(2) 86.8(3), O(2)–Ni–O(2) 86.2(2), O(1)–Ni–N(2) 94.6(2) and O(1)–Ni–N(1) 169.9(2). These results are consistent with similar Ni(II) complexes [17, 30]. In the crystal packing system, two types of short interactions were detected: 2H-bonds C-H....O of 2.433 Å and 2H..., C = C bonds of 2.665 Å.

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Bond no.	Bonds (Å)		Exp. XRD	DFT/B3LYP	Angle no.	Angles (°)			Exp. XRD	DFT/B3LYP
1	Ni1	01	1.834(5)	1.8051	1	01	Ni1	02	86.2(2)	88.8
2	Ni1	02	1.838(5)	1.8068	2	01	Ni1	N7	169.9(2)	163.58
3	Ni1	N7	1.849(6)	1.7762	3	01	Ni1	FN8	94.6(2)	94.03
4	Ni1	N8	1.836(6)	1.7866	4	02	Ni1	N7	94.0(2)	93.37
5	01	C3	1.318(7)	1.3252	5	02	Ni1	N8	171.4(2)	163.27
6	02	C4	1.312(7)	1.3272	6	N7	Ni1	N8	86.8(3)	88.57
7	C3	C5	1.442(9)	1.438	7	Ni1	01	C3	129.4(4)	131.01
8	C3	C6	1.39(1)	1.4253	8	Ni1	02	C4	128.5(4)	131.2
9	C4	C13	1.42(1)	1.4292	9	01	C3	C5	119.9(6)	121.28
10	C4	C16	1.438(9)	1.434	10	01	C3	C6	121.5(6)	121.19
11	C5	C14	1.389(8)	1.3842	11	C5	C3	C6	118.5(6)	117.54
12	C5	C25	1.52(1)	1.5391	12	02	C4	C13	122.5(6)	121.22
13	C6	C11	1.43(1)	1.4182	13	02	C4	C16	119.0(6)	121.41
14	C6	C24	1.43(1)	1.4212	14	C13	C4	C16	118.6(6)	117.37
15	N7	C9	1.29(1)	1.3115	15	C3	C5	C14	117.8(6)	118.39
16	N7	C22	1.486(9)	1.4867	16	C3	C5	C25	120.3(5)	120.23
17	N8	C24	1.30(1)	1.312	17	C14	C5	C25	121.9(6)	121.38
18	N8	C32	1.493(9)	1.5162	18	C3	C6	C11	119.8(6)	121.46
19	C9	C13	1.40(1)	1.4209	19	C3	C6	C24	122.3(6)	120.01
20	C10	C16	1.392(8)	1.3886	20	C11	C6	C24	117.9(6)	118.52

Table 3. Selected exp. XRD and DFT-B3LYP bond lengths and angles.



Figure 2. (a) XRD/DFT bonds distances relation, (b) bonds distances graphical correlation, (c) DFT/ XRD angles relation and (d) angles graphical correlation.

Very good agreement between DFT/XRD bond distances and angles were observed as shown in Figure 2(a,c), respectively. The bond lengths graphical correlation (R^2) was found to be 0.982 (Figure 2(b)), whereas the angles graphical correlation (R^2) was found to be 0.9907 (Figure 2(d)). In general, significant matching between XRD/DFT structural parameters was observed.

3.3. HSA, FP and MPE computation

Figure 3 elucidates the molecular interactions in the **NiL** complex with the aid of HSA and FP calculations using the CIF. The result was compared with the XRD-packing result [38–43]. HSA reflects the presence of 2 red points around O atoms (Figure 3(a)), indicating the H-O....H and H....C=C bonds connected the **NiL** complex lattice in layer-by-layer diminutions. This finding supported the XRD-packing result. The percentages ratio of atom...atom FP contacts are ordered as H-H(82.0%)>H-C>H-O>H-N and H-Ni (<0.4%), as shown in Figure 3(d).

The MEP created in space around the **NiL** complex by the charge allocation is useful in showing the interacting sites for an electrophilic and nucleophilic hit in the biological system. The MEP result of the **NiL** complex strongly supports the HSA and XRD results. The different electrostatics potential values are presented by various colors; blue represents the positive region of electrostatic potential that is due to CH₂ in the diamine ligand part. The red color reflected the high electrostatic potential that is around e-rich O atoms only. The green color represents less positive potential regions in the complex. MEP suggests the HCH ... O hydrogen bond and HCH ... π C = C bonds can be formed via the interaction between the e-rich (2 O) with e-poor (CH₃, CH₂ and = CH) functional groups [40–44]. This observation is matched with the XRD and HSA results (Figure 4).

3.4. Infra-red studies of H₂L ligand and NiL complex

Several functional groups such as C_{sp}^{3} -H, C_{sp}^{2} -H C = N, C = C, C-O, C-C, Ni-O and Ni-N were detected by FT-IR, theoretically and experimentally as shown in Figure 5. Noticeably, the B3LYP-IR frequencies of the main functional groups in the gaseous sate are higher than those experimentally observed for the equivalent groups, in solid state. The Exp./DFT IR are in high agreement as seen by the 0.998 correlation coefficient shown in Figure 5. The solid state infrared spectrum of the free H₂L exhibits no broad band for the pronounced OH vibration in the region of $3410-3450 \text{ cm}^{-1}$, probably due to the strong (O-H...N=C) intra-molecular hydrogen bonding [44]. Therefore, the undistinguished broad band of the OH in the free H_2L is not helpful in confirming Ni coordination. However, coordination of the free ligand with the Ni center can be confirmed by two other options. The chemical shift of the azomethine C = N group in the complex shifted to lower energy by 17 units (1612 cm⁻¹) when compared to the same azomethine group in the free ligand (1629 cm^{-1}) , as can be seen in Figure 5(a). The Ni-O and Ni-N exhibit a broad peak at 540 cm^{-1} in the spectrum of the complex, indicating a coordination mode through these two atoms as shown in Figure 5(b) [28]. The DFT-IR for NiL was performed for comparison. The study shows several functional groups consistent with the complex structure (Figure 5).

3.5. UV-Vis

UV-Vis behaviors of both free **H**₂**L** ligand and its **NiL** complex were compared in ethanol (Figure 6). The $\pi \rightarrow \pi^*$ electron transfer **H**₂**L** ligand bands were observed at 277 nm



Figure 3. Hirshfeld surfaces views for the NiL complex (a) d_{norm} (b) shape index, (c) curvedness structures and (d) inside/outside 2 D-FP plot.

and 335 nm, whereas in the **NiL** complex these bands were shifted slightly to lower energy 280 nm and 342 nm, respectively. These shifts confirm formation of the new Ni-N and Ni–O bonds. The new MLCT broadband appeared only in the **NiL** complex (at 425 nm), supporting the formation of square planar geometry around the Ni center (Figure 6(b)).

3.6. Thermal gravimetric analysis

TG/DSC analysis of the **NiL** complex showed one stage of decomposition pattern with heating rate of $10 \degree \text{C} \text{ min}^{-1}$ in the 25 to $800 \degree \text{C}$ temperature range and air atmosphere (Figure 7). Below 260 °C, the **NiL** complex displayed significant thermal stability; no



Figure 4. MEP map of NiL complex.



Figure 5. Exp. IR spectra of (a) free H_2L ligand, (b) NiL complex, (c) DFT/B3LYP/6-311G(d) of NiL and (d) DFT/Exp. correlation coefficient.



Figure 6. UV-vis spectra of free H₂L (a) and NiL complex (b) dissolved in ethanol.



Figure 7. TG/DSC curves.

loss of water or other solvent molecules in the complex lattice were observed. This observation is in agreement with the IR and XRD results. The ligand **ONNO** was thermally destructured from the **NiL** through a broad one step in ~280–450 °C with two $T_{DSC} = 305$ and 318 °C. The organic content completely decomposed parallel to NiO formation with 12.5% as a final product; the NiO final product was confirmed by IR [45].

4. Conclusion

In this study, the X-ray crystallography study confirms the structure of a newly synthesized Ni complex. The Schiff base acts as a single tetradentate ONNO chelating agent through the azomethine nitrogen atoms and the phenolic oxygen atoms. It shows a Ni^{II} center with slightly distorted square planar geometry. Moreover, a sufficient number of H-bonds and H... π stacks stabilized the lattice. Electrostatic potential surface (MEP) and Hirschfeld surface analysis (HSA) were found to be in good agreement with the corresponding experimental data. The DFT-optimized **NiL** reflected significant thermal stability and it decomposed in open atmosphere in a one-step thermal decomposition process.

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Disclosure statement

No potential conflict of interest was reported by the authors.

References

- [1] S. Chatterjee, D. Sukul, P. Banerjee, J. Adhikary. Inorg. Chim. Acta, 474, 105 (2018).
- [2] D. Çakmak, S. Çakran, S. Yalçinkaya, C. Demetgül. J. Electroanal. Chem, 808, 65 (2018).
- [3] L.H. Abdel-Rahman, N.M. Ismail, M. Ismael, A.M. Abu-Dief, E.A.-H. Ahmed. J. Mol. Struct., 1134, 851 (2017).
- [4] N. Kavitha, P.V. Anantha Lakshmi. J. Saudi Chem. Soc., 21, S457 (2017).
- [5] Y. Jia, J. Li. Chem. Rev., **115**, 1597 (2015).
- [6] C.J. Reda, F.M. Elshaarawy, Z.H. Kheiralla, A.A. Rushdy, C. Janiak. *Inorg. Chim. Acta*, **421**, 110 (2014).
- [7] M.S.S. Adam, L.H. Abdel-Rahman, A.M. Abu-Dief, N.A. Hashem. *Inorg. Nano-Met. Chem.*, 50, 132 (2020).
- [8] K. Jana, S. Das, H. Puschmann, S.C. Debnath, A. Shukla, A.K. Mahanta, M. Hossain, T. Maity, B.C. Samanta. *Inorg. Chim. Acta*, 487, 128 (2019).
- [9] M.M. Mostafa, K.M. Ibrahim, M.N.H. Moussa. Trans. Met. Chem., 9, 243 (1984).
- [10] M. Salehi, M. Hasanzadeh. Inorg. Chim. Acta, 426, 6 (2015).
- [11] M. Gupta, V. Kumar Vaidya. Int. Res. J. Pharm. Med. Sci., 2, 36 (2019).
- [12] M.S. Altowyan, A. Barakat, A.M. Al-Majid, H.A. Ghabbour, A. Zarrouk, I. Warad. BMC Chem, 13, 1 (2019).
- [13] P.G. Cozzi. Chem. Soc. Rev., 33, 410 (2004).
- [14] G.P. Wu, W.M. Ren, Y. Luo, B. Li, W.Z. Zhang, X.B. Lu. J. Am. Chem. Soc., 134, 5682 (2012).
- [15] F. Kratz, U. Beyer, M.T. Schütte. Crit. Rev. Ther. Drug Carrier Syst., 16, 245 (1999).
- [16] H. Saito, A.S. Hoffman, H.I. Ogawa. J. Bioact. Compat. Polym., 22, 589 (2007).
- [17] N. Charef, F. Sebti, L. Arrar, M. Djarmouni, N. Boussoualim, A. Baghiani, S. Khennouf, A. Ourari, M.A. AlDamen, M.S. Mubarak, D.G. Peters. *Polyhedron*, **85**, 450 (2015).
- [18] P.K. Sasmal, A.K. Patra, A.R. Chakravarty. J. Inorg. Biochem., 102, 1463 (2008).
- [19] K. Dhahagani, S. Mathan Kumar, G. Chakkaravarthi, K. Anitha, J. Rajesh, A. Ramu, G. Rajagopal. Spectrochim. Acta, Part A, 117, 87 (2014).
- [20] L. Peng, C. Chen, C.R. Gonzalez, V. Balogh-Nair. Int. J. Mol. Sci., 3, 1145 (2002).
- [21] H. Keypour, M. Ahmadi, M. Rezaeivala, A. Chehregani, R. Golbedaghi, A.G. Blackman. Polyhedron, 30, 1865 (2011).
- [22] A. Choudhary, R. Sharma, M. Nagar. Int. Res. J. Pharm. Pharmacol., 1, 2251 (2011).
- [23] S. Matsunaga, M. Shibasaki. Chem. Commun., 50, 1044 (2014).
- [24] Z. Liu, F.C. Anson. Inorg. Chem., 40, 1329 (2001).
- [25] S.N. Shukla, P. Gaur, M.L. Raidas, B. Chaurasia. J. Mol. Struct., 1202, 127362 (2020).
- [26] Z.M. Bikbaeva, D.M. Ivanov, A.S. Novikov, I.V. Ananyev, N.A. Bokach, V. Yu. Kukushkin. Inorg. Chem., 56, 13562 (2017).
- [27] D.S. Bolotin, Z.M. Bikbaeva, A.S. Novikov, V.V. Suslonov, N.A. Bokach. Chem. Select., 15, 9669 (2017).
- [28] A.D. Garnovskii, A.L. Nivorozhkin, V.I. Minkin. Coord. Chem. Rev., 126, 1 (1993).
- [29] C.T. Cohen, C.M. Thomas, K.L. Peretti, E.B. Lobkovsky, G.W. Coates. *Dalton Trans.*, **60**, 237 (2006).
- [30] W.K. Dong, Y.X. Sun, G.H. Liu, L. Li, X.Y. Dong, X.H. Gao. Z. Anorg. Allg. Chem., 638, 1370 (2012).

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- [31] M.A. Turner, J.J. McKinnon, S.K. Wolff, D.J. Grimwood, P.R. Spackman, D. Jayatilaka, M.A. Spackman. *CrystalExplorer, Version* 17, University of Western Australia, Perth (2017).
- [32] D.J. Frisch, J. Trucks, G.W. Schlegel, H.B. Scuseria, G.E. Robb, M.A. Cheeseman, J.R. Scalmani, G. Barone, V. Mennucci, B. Petersson, G.A. Nakatsuji, H. Caricato, M. Li, X. Hratchian, H.P. Izmaylov, A.F. Bloino, J. Zheng, G. Sonnenberg. J. Revis. A.1. M. Gaussian, Inc., Wallingford, CT (2009).
- [33] A.P.E.X. Bruker. SAINT-plus and SADABS, Bruker AXS Inc., Madison, WI (2004).
- [34] G.M. Sheldrick. Acta Crystallogr. A Found. Crystallogr., 64, 112 (2008).
- [35] G.M. Sheldrick. Acta Crystallogr. A Found. Adv., 71, 3 (2015).
- [36] A.L. Spek. Acta Crystallogr. D Biol. Crystallogr., 65, 148 (2009).
- [37] C.F. Macrae, I.J. Bruno, J.A. Chisholm, P.R. Edington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek, P.A. Wood. J. Appl. Crystallogr., 41, 466 (2008).
- [38] A. Titi, T. Shiga, H. Oshio, R. Touzani, B. Hammouti, M. Mouslim, I. Warad. J. Mol. Struct., **1199**, 1 (2020).
- [39] M.R. Aouad, M. Messali, N. Rezki, N. Al-Zaqri, I. Warad. J. Mol. Liq., 264, 621 (2018).
- [40] A. Barakat, M.S. Islam, A.M. Al-Majid, H.A. Ghabbour, S. Atef, A. Zarrouk, I. Warad. J. Theor. Comput. Chem., 17, 1850005 (2018).
- [41] F.A. Saleemh, S. Musameh, A. Sawafta, P. Brandao, C.J. Tavares, S. Ferdov, A. Barakat, A.A. Ali, M. Al-Noaimi, I. Warad. *Arab. J. Chem.*, **10**, 845 (2017).
- [42] I. Warad, F.F. Awwadi, B. Abd Al-Ghani, A. Sawafta, N. Shivalingegowda, N.K. Lokanath, M.S. Mubarak, T. Ben Hadda, A. Zarrouk, F. Al-Rimawi, A.B. Odeh, S.A. Barghouthi. *Ultrason. Sonochem.*, 48, 1 (2018).
- [43] M.R. Aouad, M. Messali, N. Rezki, M.A. Said, D. Lentz, L. Zubaydi, I. Warad. J. Mol. Struct., 1180, 455 (2019).
- [44] R. Mathammal, K. Sangeetha, M. Sangeetha, R. Mekala, S. Gadheeja. J. Mol. Struct., **1120**, 1 (2016).
- [45] A. Barakat, M. Al-Noaimi, M. Suleiman, A.S. Aldwayyan, B. Hammouti, T.B. Hadda, S.F. Haddad, A. Boshaala, I. Warad. Int. J. Mol. Sci., 14, 23941 (2013).