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New coordination insights into paracetamol and 1,10-phenanthroline metal complexes: Synthesis, characterization, DFT calculations, and antimicrobial study

Zaynab. H. Alkhafagi[1], Ali J. Al-Sarray[2*], Taghreed H. Al-Noor[1], Omar H. Al-Obaidi[3], Marei El-Ajaily[4]

[1]Department of Chemistry, Ibn -Al-Haithem College of Education for Pure Science, University of Baghdad, Baghdad, Iraq
[2]Polymer Research Unit, College of Science, Mustansiriyah University, Baghdad, Iraq
[3]Chemistry Department, College of Science, University of Anbar, Iraq
[4]Department of Chemistry, Faculty of Science, University of Benghazi, Benghazi, Libya

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Corresponding author
Ali J. Al-Sarray
ali_alsarray@uomustansiriyah.edu.iq

ABSTRACT

Seven novel bidentate metal complexes of paracetamol (Para) and 1,10-Phenanthroline (Phen), with the general formula [M(Para)(Phen)2]Cl2 (M(II) = Mn, Fe, Co, Ni, Cu, Zn, and Cd), were synthesized in the present work and characterized by metal content, conductivity, melting point, elemental analysis, magnetic moment measurements, and UV-Vis and FT-IR spectroscopies. The molar conductance values further indicate that the complexes are electrolytic in nature. Paracetamol coordinates through its carbonyl (C=O) group and the amide nitrogen, whereas phenanthroline binds via its (N,N) donor atoms; therefore, both ligands act as bidentate, neutral donors. All complexes exhibit octahedral geometry, with one paracetamol and two phenanthroline ligands surrounding the metal ion. The antimicrobial activity was evaluated against two Gram-positive and two Gram-negative bacteria, as well as the fungus *Candida albicans*. DFT calculations were performed for selected complexes to obtain optimized structures and analyze electronic orbitals and related parameters.

Keywords: *1,10-Phenanthroline, Antimicrobial activity, Coordination compounds, Metal complexes, Paracetamol*

1 INTRODUCTION

Metal complexes with mixed ligands have attracted researchers' interest because of their wide range of applications in a variety of fields, including catalysis, medicine, and materials science [1–5]. In medicinal chemistry, incorporating pharmacologically active molecules into metal complexes as ligands can enhance their properties, thereby enabling them to act as new therapeutic agents [1]. Complexation can also lead to improved bioavailability, selectivity, solubility, and overall higher efficacy in comparison to the free ligand [6, 7].

Paracetamol (Para), also known as acetaminophen, is considered one of the most widely used analgesics and antipyretic drugs, with a high safety profile [8, 9]. Its mechanism of action includes inhibition of cyclooxygenase (COX) enzymes, which are responsible for producing inflammatory mediators [8]. However, the antibacterial and antifungal activities of this drug are very limited and low [9]. In contrast, 1,10-phenanthroline (Phen) is a bidentate N,N-chelating ligand that can form coordination complexes with metals and has potential biological activity [2]. Many studies have reported the efficacy of this

compound as an antibacterial agent after incorporation into complexes, specifically against *Pseudomonas aeruginosa* and its biofilms [2,10]. Moreover, other studies have suggested using Phen and its complexes as insecticidal and antiparasitic agents [3, 5]. These activities can be attributed to potential interactions of this compound and its complexes with cellular components and the disruption of related biological processes [4, 11].

Although various studies have synthesized metal complexes involving 1,10-phenanthroline and paracetamol, such as the work by Jamil et al. (2018) with Co(II), Ni(II), and Cu(II) in a 1:1:1 molar ratio [12], the biological potential of these systems remains insufficiently explored. In particular, the activity of bivalent metal complexes formed with Para and Phen ligands has not been thoroughly investigated across a broader range of metal ions and stoichiometries. In this study, we report the synthesis and characterization of a novel series of bivalent metal complexes involving Mn(II), Fe(II), Co(II), Ni(II), Cu(II), Zn(II), and Cd(II) ions in a 1:2:1 stoichiometric ratio of [M(Para)(Phen)2]Cl2. Chelation of paracetamol to metal ions is anticipated to improve target specificity and enhance cellular uptake, whereas complexation with 1,10-phenanthroline may broaden biological activity due to its known interactions with biomolecular targets [13]. The aim of the present work is to investigate the structural, spectroscopic, and electronic properties of these complexes, to evaluate their antimicrobial activities, and to employ density functional theory (DFT) calculations to model their optimized geometries and to explore associated electronic parameters.

2 MATERIALS AND METHODS

2.1 Chemicals and materials

The chemicals used in the current study were supplied by BDH, GFS, and Fluka and were used without further purification. These included paracetamol (C8H9NO2), 1,10-phenanthroline (Phen), and metal chlorides of the bivalent metals used in this study in the form of FeCl2·4H2O, MnCl2·4H2O, CuCl2·2H2O, NiCl2·6H2O, CoCl2·6H2O, ZnCl2, and CdCl2.

2.2 Characterization methods

FT-IR spectra were recorded on a Shimadzu 8300 spectrophotometer as KBr pellets, whereas magnetic susceptibility was measured at ambient temperature in the Department of Chemistry laboratory at the University of Baghdad. Elemental analysis (C, H, and N) was performed using a PerkinElmer CHN-2400 elemental analyzer. Electronic properties were investigated using UV-visible (UV-Vis) spectroscopy with a Shimadzu UV-160A spectrophotometer, analyzing 10^{-3} M complex solutions in dimethyl sulfoxide (DMSO). Atomic absorption spectroscopy was used to determine the metal content in the synthesized complexes. Finally, molar conductivity (Λm) measurements of 10^{-3} mol L^{-1} complex solutions in DMSO were obtained using an InoLab 720 digital conductivity meter.

2.3 Preparation of complexes

A similar procedure was followed for synthesizing all seven bivalent metal complexes with paracetamol (Para) and 1,10-phenanthroline (Phen). The stoichiometric ratio used was [Para: M:2Phen]. Figure 1 illustrates the general reaction for complex formation. In a typical synthesis, 2 mmol (318.2 mg) of 1,10-phenanthroline and 1 mmol (151.1 mg) of paracetamol were dissolved in a minimal amount of hot absolute ethanol (20 mL). A hot ethanolic solution (10 mL) containing 1 mmol of the corresponding metal chloride salt ($FeCl_2.4H_2O$, $MnCl_2.4H_2O$, $CuCl_2.2H_2O$, $NiCl_2.6H_2O$, $CoCl_2{\cdot}6H_2O$, $ZnCl_2$, and $CdCl_2$) was added slowly to this solution with constant stirring, followed by refluxing the reaction mixture for 4–6 h. The resulting precipitate was then filtered off while hot and washed with hot ethanol (2 × 10 mL) before drying in a desiccator over anhydrous $CaCl_2$. The yield for the complexes ranged from 84% to 92%.

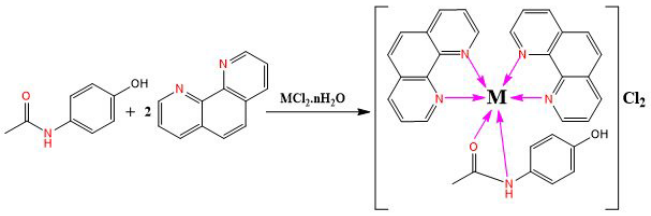

Fig. 1 Preparation of $[M(Para)(Phen)_2]Cl_2$ complexes, where M(II)= Mn, Fe, Co, Ni, Cu, Zn, and Cd

2.4 Biological activities

The in vitro antifungal and antibacterial activities of the synthesized complexes were assessed using the well-diffusion method [14]. The test microorganisms included Gram-positive bacteria (*Bacillus cereus* and *Staphylococcus aureus*), Gram-negative bacteria (*Pseudomonas aeruginosa* and *Escherichia coli*), and the fungus *Candida albicans*. Dimethyl sulfoxide (DMSO) was used as the

solvent and as a control in the experiment.

2.5 DFT calculations

DFT calculations were carried out using the B3LYP method with the 6-31G(d,p) basis set for the ligands and the LanL2DZ basis set for metal ions. The Gaussian 09 software package was used for the calculations, and GaussView was used to visualize the output. The complexes were optimized at the same level of theory used for the calculations, and the Highest Occupied and Lowest Unoccupied Molecular Orbitals (HOMO and LUMO, respectively) were obtained. From the determined molecular orbitals, other associated electronic parameters were obtained, such as the energy gap, chemical softness, chemical hardness, ionization potential, and electronic affinity [15, 16].

3 RESULT AND DISCUSSION

This study successfully synthesized and characterized a series of seven binuclear metal complexes containing paracetamol (Para) and 1,10-phenanthroline (Phen) ligands with bivalent metal ions (M(II) = Mn, Fe, Co, Ni, Cu, Zn, and Cd). In this work, the synthesized complexes were examined using multiple analytical approaches. The 1:2:1 stoichiometry of [M(II):Para:2Phen] employed in the synthesis was achieved, as evidenced by the good agreement between the experimental and calculated formula weights of the complexes (Table 1). The melting points provide valuable insights into the thermal behavior of these newly synthesized complexes. Notably, the complexes' insolubility in various solvents, including water and common organic solvents (DMSO, hexane, ethanol, benzene, acetone, and methanol), as well as in HCl, suggests unique physicochemical properties. This insolubility may be attributed to strong interactions between the metal ion and the ligand molecules, resulting in a neutral coordination complex.

3.1 Characterization

Further characterization employed atomic absorption spectroscopy (AAS) to determine the metal content within the complexes. The satisfactory agreement between the experimental and calculated values of metal percentages in Table 1 reinforces successful incorporation of the targeted metal ions in the desired stoichiometry. Additionally, the presence of chloride counterions (Cl^-) outside the coordination sphere was confirmed by a positive test with $AgNO_3$ solution for all complexes. This supports the overall charge neutrality of the complexes, with two chloride ions balancing the positively charged metal ion (M^{2+}).

A crucial aspect of the characterization involved measuring the molar conductivity of the complexes in DMSO solution. The observed high molar conductivities for all complexes (except the Cu(II) complex) provide significant insights into their electrolytic behavior in solution under the measurement conditions. These values suggest that the complexes dissociate into ions when dissolved in DMSO, likely existing as 1:2 electrolytes consistent with the proposed formula [M(Para)(Phen)2]Cl_2. This dissociation behavior implies potential ionic mobility of the complexes in a polar environment, which could be relevant for their biological activity or other applications [17].

To investigate the effect of complexation on ligand functional-group frequencies, as well as newly formed bonds between the metal ions and the ligands' donor atoms, FT-IR spectra were recorded for the prepared complexes (Table 2) to support these assignments and comparisons. The FT-IR spectra showed the disappearance and shifts of certain ligand functional groups, indicating coordination of the ligands to the metal ions. The carbonyl ν(C=O) band shifted to lower frequencies due to changes in the electronic environment around the C=O group upon complexation. Similarly, frequency shifts were observed in the ν(N–H) and ν(C=N) bands of the complexes compared with the free ligands. These shifts suggest that the nitrogen of the amino group and the oxygen of the carbonyl group of the paracetamol ligand, as well as the nitrogen of the C=N group of 1,10-phenanthroline, are involved in coordination with the metal ions. Furthermore, the appearance of the ν(M–O) and ν(M–N) bands supports coordination between the ligands and metal ions [18].

The magnetic moments of all complexes showed paramagnetic behavior, except for the Zn(II) and Cd(II) complexes, which showed diamagnetic behavior [19]. Table 3 lists the calculated data derived from the measured magnetic susceptibilities for these complexes. However, the UV-Vis spectrum of the Phen ligand exhibits one electronic peak at 289 nm (34,602 cm^{-1}), which is due to a $\pi \rightarrow \pi^*$ transition. The electronic spectra of the prepared complexes revealed two types of electronic transitions. LMCT transitions, observed in all complexes, are responsible for their colors. In addition, d–d transitions were observed for complexes containing partially filled d orbitals (Mn, Fe, Co, Ni, and Cu) within a

Table 1 Analytical and compositional data of the prepared complex

Comp.	Color	M. Wt. (g/mol)	m.p. (°C)	M% (Exp.)	Λm ($\Omega^{-1}cm^2$ mol^{-1}) (DMSO)	C% (Theo.)	H% (Theo.)	N% (Theo.)
[Mn(Para)(Phen) $_2$] Cl_2	White	637.52	>260	6.68	7.6	60.23 (60.30)	3.92 (3.95)	10.98 (10.99)
[Fe (Para)(Phen) $_2$] Cl_2	Red	636.85	>260	7.31	86.26	60.29 (60.36)	3.21 (3.96)	10.99 (11.00)
[Co(Para)(Phen)$_2$] Cl_2	Green	639.9	>260	7.8	70.4	60.00 (60.05)	3.90 (3.94)	10.93 (10.95)
[Ni (Para)(Phen) $_2$] Cl_2	Green	639.6	>260	7.77	69.85	60.03 (60.09)	3.90 (3.94)	10.94 (10.95)
[Cu(Para)(Phen)$_2$] Cl_2	Blue	644.5	>260	8.36	8.33	59.58 (59.64)	3.87 (3.91)	10.86 (10.87)
[Zn(Para)(Phen)$_2$] Cl_2	White	648.3	>260	8.58	73.51	59.23 (59.29)	3.86 (3.89)	10.83 (10.81)
[Cd(Para)(Phen)$_2$] Cl_2	White	693	>260	13.89	91.15	55.37 (55.46)	3.60 (3.64)	10.09 (10.11)

Note. m.p.: Melting Point, M. Wt.: Molecular Weight, M% (Exp.): Experimental Metal Content (%), Λm: Molar Conductivity, and (Theo.): Theoretical Value

Table 2 Recorded FT-IR frequencies of the main functional groups of the prepared complexes

Complex	ν(O − H)ν(N − H)	ν(C − H) arom.	ν(C = O)	ν(C = N)	ν(C − O)	ν(M − N)	ν (M-O)
[Mn(Para)(Phen)$_2$] Cl_2	3414	3059	1627	1512	1249	567	478
[Fe (Para) (Phen)$_2$] Cl_2	3321	3051	1624	1512	1273	578	439
[Co(Para)(Phen)$_2$] Cl_2	3425 3373	3051	1624	1512	1257	524	451
[Ni (Para)(Phen) $_2$] Cl_2	3321	3051	1624	1512	1257	570	451
[Cu(Para)(Phen)$_2$] Cl_2	3441	3059	1624	1561	1222	574	466
[Zn(Para)(Phen)$_2$] Cl_2	3448	3047	1620	1570	1222	561	474
[Cd(Para)(Phen)$_2$] Cl_2	3444, 3479 Vs	3047	1624	1512	1222	555	459

range of 10,604–23,752 cm^{-1}. Notably, the Cd(II) and Zn(II) complexes lacked d–d transitions because of their complete d-electron configurations [20].

The spectrum of [Mn(Para)(Phen)2]Cl2 showed three main peaks (Figure 2a): two peaks at 275 nm (36,363 cm^{-1}) and 290 nm (34,482 cm^{-1}) due to the LMCT transition, and another band at 881 nm (13,850 cm^{-1}) due to the 6A1g(S)→4T2g(G) d-d transition. The μeff value of the Mn(II) complex (5.13 B.M.) agrees with another study of the [Mn(phen)(Val)2] complex, which showed 5.13 B.M. [21], suggesting a high-spin d5 Mn(II) ion in Oh geometry.

The spectrum of [Fe(Para)(Phen)2]Cl2 exhibits three peaks, as shown in Figure 2b, which are due to d-d transitions: 517 nm (19,342 cm^{-1}) due to 6A1g(S)→4T1g, 900 nm (11,111 cm^{-1}) ascribed to 6A1g(S)→4T2g, and 943 nm (10,604 cm^{-1}) ascribed to 5T2g→5Eg. The spectrum of the Co(II) complex showed several peaks (Figure 2c), including 290 nm (34,482 cm^{-1}), attributed to CT, and two peaks at 533 nm (18,761 cm^{-1}) and 810 nm (12,345 cm^{-1}), attributed to 4T1g→4T1g(P) and 4T1g→4A2g(F) transitions, respectively [19]. The Ni(II) complex spectrum exhibited three peaks (Figure 2d), including 421 nm (23,752 cm^{-1}), 515 nm (19,417 cm^{-1}), and 737 nm (13,568 cm^{-1}), attributed to d-d transitions of 3A2g(F)→3T1g(P), 3A2g(F)→3T1g(F), and 3A2g(F)→3T2g(F), respectively [22]. The spectrum of [Cu(Para)(Phen)2]Cl2 (Figure 2e) exhibited two peaks: a high-intensity peak at 297 nm (33,670 cm^{-1}), ascribed to CT, and a second, weak-intensity peak in the visible region at 749 nm (13,351 cm^{-1}), attributed to the (2Eg→2T2g) transition [21]. The blue Cu(II) complex has μeff of 1.61 B.M., which corresponds to its octahedral structure [23, 24].

These spectral data, together with the magnetic moment data, strongly support the proposed octahedral geometries for all complexes except for Cd(II) and Zn(II). The absence of paramagnetic behavior in these two complexes suggests that the metal ions (Cd^{2+} and Zn^{2+}) have filled d-electron configurations, and their geometries might deviate from the typical octahedral structure. Further investigations, such as X-ray crystallography, could be employed in future work to definitively determine the exact geometries of these complexes.

3.2 Biological activity

This study explored the potential biological activity of the synthesized complexes by evaluating their in vitro antifungal and antibacterial activities against a panel of commonly encountered microbial strains. The results (Figure 3) revealed some trends. The free paracetamol ligand exhibited negligible antibacterial and antifungal activities, indicating that the ligand alone is not effective against the tested bacteria and fungi, whereas 1,10-phenanthroline showed excellent antibacterial and antifungal activities. In general, the complexes

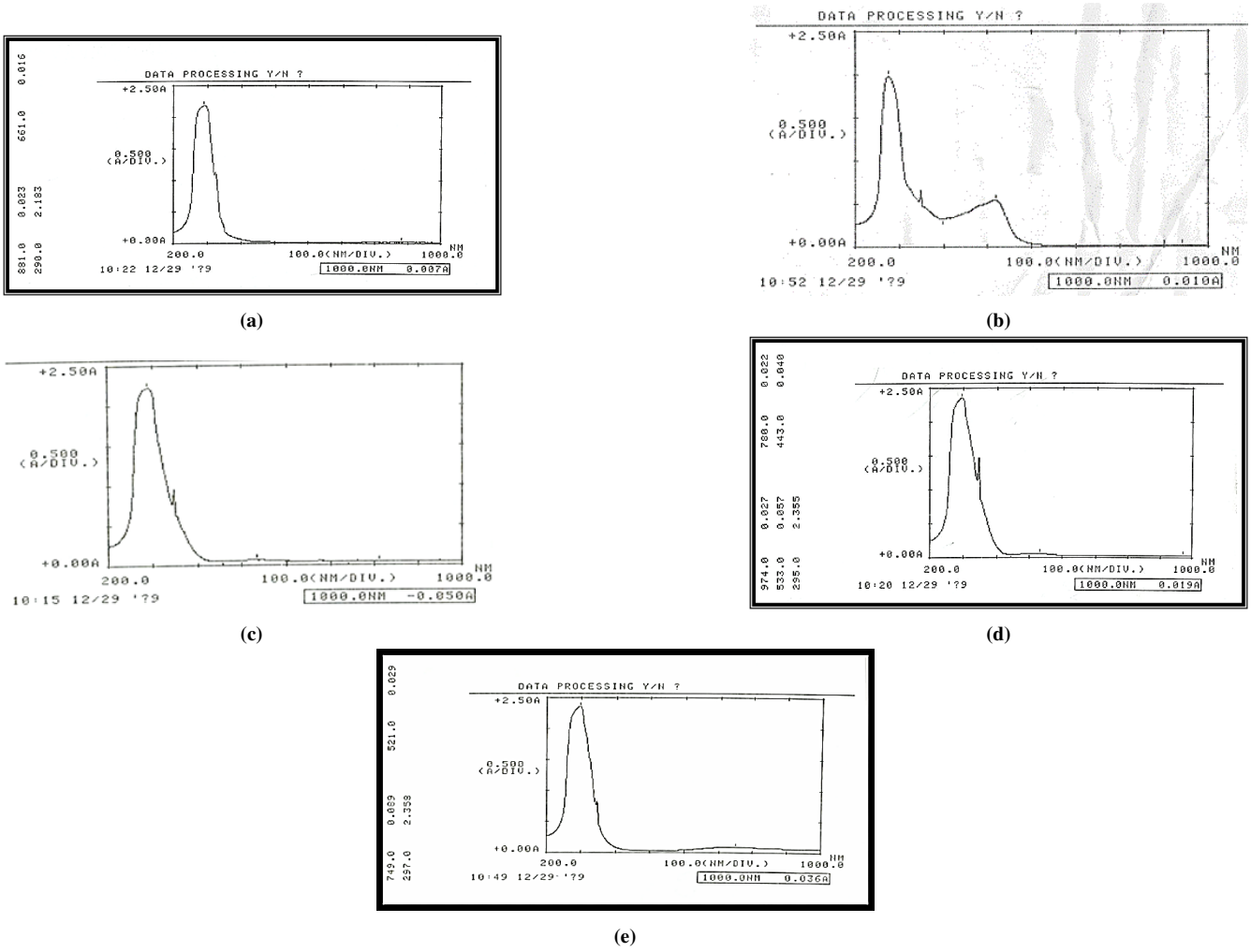

Fig. 2 Electronic spectra of prepared M(II) complexes of (a) Mn, (b) Fe, (c) Co, (d) Ni, and (e) Cu metal ions

exhibited much higher activity compared with the free Para ligand, suggesting that complexation with the Phen ligand can elevate the biological activity of the Para ligand. Differences in biological activity were observed among the complexes depending on the metal ions used. The [Cu(Para)(Phen)2]Cl2 complex showed the highest antifungal activity against *Candida albicans*, which might be attributed to the redox properties of Cu(II) ions that generate reactive oxygen species (ROS) that destroy microbial cells [5]. Furthermore, the Mn(II) and Cd(II) complexes exhibited very high antibacterial activity against Gram-positive bacterial strains, which is most probably attributed to the chelating effect between the ligands and the metal ions, increasing the lipophilic character of the complexes and aiding their penetration through the cell membrane [13, 25].

3.3 DFT study

Figure 4 shows the optimized structures of the Ni(II) and Mn(II) complexes that were studied using density functional theory with the B3LYP method and the 6-31G(d,p) basis set for the ligands and the LanL2DZ basis set for the metals [11]. The HOMO and LUMO molecular orbitals were calculated according to the described methods to obtain the electronic parameters for the complexes. The band gap values for the studied complexes were small, indicating high activity. The Mn(II) complex showed a lower value (1.423 eV) (Figure 5b) compared with the Ni(II) complex (1.442 eV) (Figure 5a), which suggests a higher activity for the Ni(II) complex. Table 4 illustrates the electronic parameters associated with HOMO and LUMO values, which showed very promising potential and activities for the studied complexes [1].

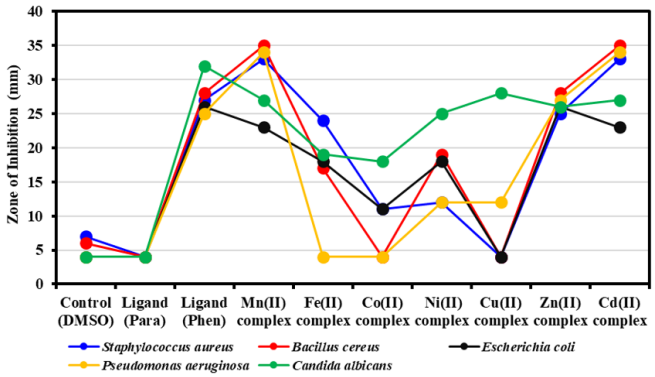

Fig. 3 Biological activity of the prepared complexes

Table 3 Comparison of Classification Results.

Parameter	HOMO	LUMO	AE	Ip	EA	μ	η	χ	ω	σ
Ni(II)comp.	-9.524	-8.082	1.442	9.524	8.082	-8.803	0.721	8.803	4.401	1.387
Mn(II)comp.	-9.894	-8.471	1.423	9.894	8.471	-9.182	0.712	9.182	4.591	1.405

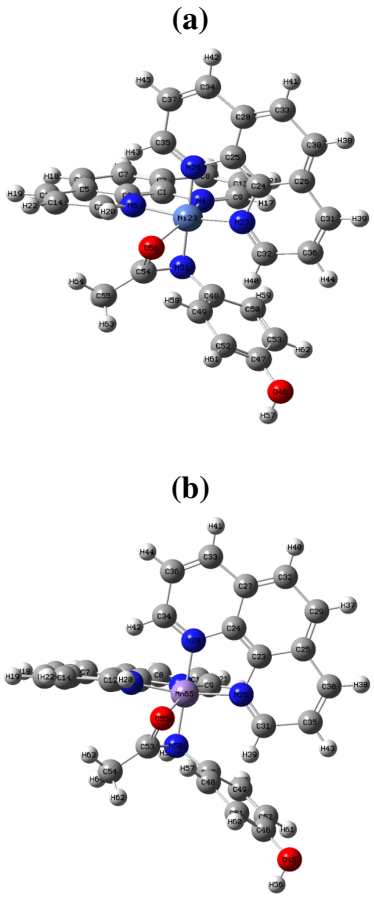

Fig. 4 The optimized structures of the prepared M(II) complexes of (a) Ni and (b) Mn metal ions

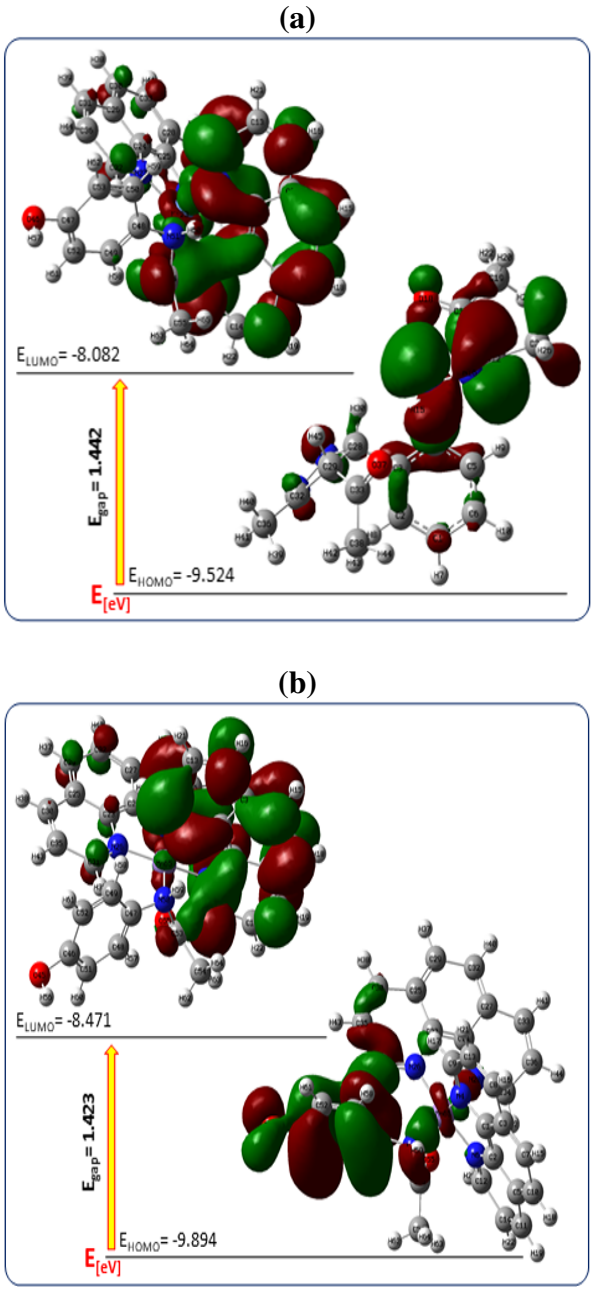

Fig. 5 HOMO, LUMO, and Energy gap for (a) Ni(II) and (b) Mn(II) complexes.

4 CONCLUSION

This study successfully achieved the synthesis and characterization of a series of seven binuclear metal complexes containing paracetamol and 1,10-phenanthroline ligands with bivalent metal ions. Analytical data confirmed formation of the complexes in the anticipated 1:2:1 stoichiometry (M:Para:Phen). FT-IR spectroscopy

provided evidence for coordination of both paracetamol and 1,10-phenanthroline to the metal centers. Molar conductivity measurements revealed the electrolytic nature of the complexes in DMSO solution. Electronic absorption spectroscopy and magnetic moment studies supported the proposed octahedral geometry for most complexes, with Cd(II) and Zn(II) potentially possessing different geometries because of their filled d-electron configurations. The most significant finding was the enhanced antibacterial activity observed for the metal complexes compared with free paracetamol, highlighting the potential of complexation to improve the bioactivity of paracetamol. In addition, the Cu(II) complex demonstrated the most potent antifungal activity. DFT calculations were carried out for the Mn(II) and Ni(II) complexes, which showed the highest activity for the Mn(II) complex because it has the lowest gap-energy value, in good agreement with the experimental findings.

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Data availability

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DECLARATIONS

Conflict of interest

The authors declare no competing interests

Consent to publish

N/A

Ethical approval

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