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Synthesis, Characterization, and in Silico ADMET Evaluation of Transition Metal Complexes Based on Ortho-Phenylenediamine and Its Derivatives

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Abstract: A series of cobalt (II), nickel (II), and zinc(II) complexes were synthesized using ortho-phenylenediamine and its two substituted derivatives (methyl- and nitro-ortho-phenylenediamine) as ligands. These complexes were isolated and characterized using various analytical techniques, including Elemental analysis, infrared (IR) and UV-Visible spectroscopy, gravimetry, and conductimetry. Conductimetric analysis revealed that all the complexes exhibit a non-electrolytic behavior in solution, indicating the absence of free ions in the medium. IR spectroscopic studies allowed the identification of the coordination modes of the ligands to the metal centers. Comparison of the IR spectra of the complexes with those of the free ligands highlighted the involvement of the amine ($-NH_2$) groups in coordination with the metal, confirming their role as the primary coordination sites. UV-Visible spectroscopic analysis was used to determine the geometry of the complexes. The observed absorption bands are characteristic of an octahedral coordination around the metal ions, which is consistent with the expected electronic transitions for these systems. In recent years, the integration of computational methodologies has considerably enhanced the ability to predict the toxicity and pharmacokinetic behavior of bioactive compounds, thereby streamlining the early stages of drug discovery. Within this framework, the present study investigates the ADMET profiles - Absorption, Distribution, Metabolism, Excretion, and Toxicity as well as the drug-likeness properties of the synthesized ligands and their corresponding transition metal complexes.

Keywords: Ortho-phenylenediamine derivatives, Transition metal, ADMET properties

Introduction

The synthesis of coordination complexes involving transition metals such as nickel (II), cobalt (II), and zinc (II) and aromatic diamine ligands has garnered significant attention due to their diverse structural motifs and broad range of potential applications in catalysis, materials science, sensing, and bioinorganic chemistry (Coropceanu, 2012). These metals are particularly attractive: Nickel(II) is widely used in hydrogenation and cross-coupling catalysis, cobalt(II) exhibits promising magnetic and redox properties, and zinc(II) plays a vital role in biological systems and luminescent materials.

In this context, a series of Ni(II), Co(II), and Zn(II) complexes were synthesized using ortho-phenylenediamine (OPD) and its two substituted derivatives methyl-ortho-phenylenediamine (MOPD) and nitro-ortho-phenylenediamine (Nitro-OPD) as bidentate ligands (Bhagat, 2018). These ligands, characterized by their nitrogen donor atoms, facilitate the formation of stable chelate rings upon coordination with metal ions. The introduction of electron-donating (methyl) and electron-withdrawing (nitro) substituents on the OPD framework allows for a systematic investigation into how electronic effects influence the coordination behavior, geometry, and physicochemical properties of the resulting metal complexes. Such studies contribute to a deeper understanding of structure-property relationships in coordination compounds and support the development of metal-based functional materials with tailored applications.

Method

Physical Measurements

Elemental microanalyses were carried out at the Central Service of Analysis (CNRS,Solaize-Lyon, France). Melting points of the synthesized compounds were determined using the appropriate apparatus. The molar conductance of the complexes (10^{-3} M) in DMSO at 25 °C was measured using a CD2005 SELECTA Conductivity Meter, FTIR spectra were obtained with a PerkinElmer 65 spectrophotometer, employing the KBr tablet method, over a range of 4000–400 cm^{-1}. Electron absorption spectra were recorded with a JASCO V-630 spectrophotometer (200–1100 nm).

Synthesis of the Complexes

The metal complexes $[M(L)_2(NO_3)_2]$ (where M = Co^{2+}, Ni^{2+}, Zn^{2+} and L = OPD, MOPD, or Nitro-OPD) were synthesized under various conditions. For the cobalt-based complexes $[Co(OPD)_2(NO_3)_2]$ and $[Co(MOPD)_2(NO_3)_2]$, 0.15 g (0.5 mmol) of cobalt(II) nitrate hexahydrate and 0.11 g (1 mmol) of ortho-phenylenediamine or 4-methyl-ortho-phenylenediamine were added to 20 mL of ethanol in a beaker and stirred at approximately 50°C. As no precipitate formed, NaOH (2 M) was added dropwise until the pH reached 10, yielding a black powder after 30 minutes of stirring.

The $[Co(Nitro\text{-}OPD)_2(NO_3)_2]$ complex was synthesized by mixing 0.15 g of cobalt nitrate hexahydrate with 0.15 g of 4-nitro-ortho-phenylenediamine, followed by the addition of 20 mL of acetonitrile. The mixture was stirred at room temperature, and a few drops of concentrated HCl were added to reach pH 1.5, resulting in an immediate light orange precipitate after 30 minutes.

For the nickel complexes, a similar method was used. 0.15 g of nickel nitrate hexahydrate and 0.11 g of the ligand (OPD or MOPD) were dissolved in 20 mL of ethanol under cold stirring. The reaction with MOPD gave a light violet precipitate directly, while OPD required pH adjustment to 10 using NaOH to induce precipitation. Both were collected after 30 minutes, washed with ethanol, and air-dried.

The $[Ni(Nitro\text{-}OPD)_2(NO_3)_2]$ complex was prepared by mixing 0.15 g of nickel nitrate and 0.15 g of Nitro-OPD in 20 mL of acetonitrile. As no solid appeared, concentrated HCl was added to pH 1.5, and a beige precipitate formed after 20 minutes of stirring. For the zinc complexes, 0.15 g of zinc nitrate hexahydrate and 0.11 g of OPD or MOPD were added to 20 mL of ethanol under cold conditions. After 20 minutes, an off-white solid was obtained.

For $[Zn(Nitro\text{-}OPD)_2(NO_3)_2]$, 0.15 g of zinc nitrate in 5 mL of water was mixed with 0.15 g of Nitro-OPD in 15 mL of acetonitrile. Since no precipitate formed, NaOH was added to pH 10, yielding an orange product after 30 minutes. All precipitates were recovered by filtration, washed with the appropriate solvents (ethanol, water, or acetonitrile), and air-dried.

ADMET Prediction

Phsyicochemical properties and Pharmacokinetics Properies such as Absorption, Distribution, Metabolism, Excretion and Toxicity of all the structures were studied via admetSAR (Yang, et al., 2019)

Results and Discussions

Analyses of the Complexes

The synthesized complexes are solid and stable in air and at room temperature. They are insoluble in water, ethanol, and methanol, but show good solubility in dimethyl sulfoxide (DMSO) and dimethylformamide (DMF). The low values of molar conductivity indicate that our complexes behave as non-electrolytes. The solid-state isolated complexes and the ligands were characterized by elemental analysis, infrared (IR) spectroscopy, and UV-Visible spectroscopy. Detailed analytical and physical properties of the synthesized compounds are provided in Table 1.

Table 1. Elemental analysis data, melting points MP (°C), molar conductivity Λ ($\Omega^{-1}.cm^2.mol^{-1}$), Yield(%) of the complexes

N	Complex	Theoretical %C	Experimental %C	Th %H	Exp %H	Th %N	Exp %N	The %Metal	Exp %Metal	Λ	*MP*	Yield
1	[Co(OPD)$_2$(NO$_3$)$_2$]	38.73	38.80	4.32	4.30	22.57	22.60	19.20	19.10	28	>300	88
2	[Co(MOPD)$_2$(NO$_3$)$_2$]	39.11	39.00	4.81	4.75	16.29	16.20	19.10	19.00	25	>300	85
3	[Co(Nitro-OPD)$_2$(NO$_3$)$_2$]	29.46	29.50	2.89	2.95	22.91	23.00	19.50	19.40	15	>300	30
4	[Ni(OPD)$_2$(NO$_3$)$_2$]	38.92	39.00	4.35	4.40	22.69	22.70	20.20	20.10	23	275	92
5	[Ni(MOPD)$_2$(NO$_3$)$_2$]	39.09	39.10	4.81	4.80	16.27	16.30	20.20	20.20	16	244	52
6	[Ni(Nitro-OPD)$_2$(NO$_3$)$_2$]	29.47	29.30	2.89	2.85	22.92	22.80	20.50	20.40	16	>300	66
7	[Zn(OPD)$_2$(NO$_3$)$_2$]	38.21	38.30	4.28	4.25	22.32	22.40	22.20	22.10	25	>300	30
8	[Zn(MOPD)$_2$(NO$_3$)$_2$]	38.47	38.50	4.74	4.70	15.98	16.00	22.20	22.20	25	261	50
9	[Zn(Nitro-OPD)$_2$(NO$_3$)$_2$]	28.97	29.10	2.84	2.90	22.51	22.60	22.50	22.40	14.5	>300	30

Infrared Spect

The IR spectral analysis confirms that all three ligands (OPD, MOPD, and Nitro-OPD) coordinate to metal ions (Co^{2+}, Ni^{2+}, Zn^{2+}) through their $–NH_2$ groups, as evidenced by the shift of N–H stretching vibrations to lower wavenumbers in the complexes. Additional shifts in $C–NH_2$ and aromatic C=C bands, along with the appearance of M–N stretching bands in the 495–400 cm^{-1} region (Berradj, 2019), further support this coordination. For Nitro-OPD-based complexes, the nitro group does not participate in coordination, as its characteristic bands remain unchanged. The presence of coordinated nitrate ions is indicated by specific absorption bands in the 1400–1050 cm^{-1} region (Bougherra, 2018). All vibrational assignments are summarized in Table **2.**

UV-Vis Spectroscopy

All the spectra of the complexes show bands in the ultraviolet range between [354 and 260 nm], slightly shifted compared to those of the free ligands, confirming the complexation of the ligands to the metal. With the exception of the zinc complexes, all show a band in the range [450-360 nm]. This band is attributed to a charge transfer transition from the ligand to the metal (Shaker, 2009).

The analysis of the electronic absorption spectra of cobalt(II), nickel(II), and zinc(II) complexes reveals distinct characteristics depending on the metal's nature and coordination geometry. Cobalt(II) complexes 1 and 2 exhibit three absorption bands approximately at 540 nm, 635 nm, and 710 nm, corresponding to the electronic transitions $^4T_1g(F) \rightarrow {}^4T_1g(P)$, $^4T_1g(F) \rightarrow {}^4A_2g(F)$, and $^4T_1g(F) \rightarrow {}^4T_2g(F)$, respectively, which are indicative of an octahedral geometry.

Similarly, nickel(II) complexes 4, 5, and 6 display multiple bands in the visible region: the first around 790 nm attributed to the $^3A_2g \rightarrow {}^3T_2g(F)$ transition, the second between 554 and 643 nm corresponding to $^3A_2g \rightarrow {}^3T_1g(F)$, and the third near 512 nm associated with $^3A_2g \rightarrow {}^3T_1g(P)$, also suggesting an octahedral geometry. In contrast, zinc(II) complexes 8 and 9, due to their d^{10} electronic configuration, do not show absorption bands in the visible region but exhibit two bands in the ultraviolet region attributed to ligand-to-metal charge transfer (LMCT) transitions (Hamrani, 2017), which is consistent with an octahedral geometry.

Table 2. Characteristic IR bands of the complexes (cm^{-1})

Complex	$\nu_{as}(NH_2)$ $\nu_s(NH_2)$	$\delta(NH_2)$	$\nu(C\text{-}NH_2)$	$\nu(C=C)$ arom	$\delta(CH_3)$	$\nu(NO_2)$	Anion X (NO_3^-)	ν (M-N)
1	3350 3180	1610	1250	1460	--	--	1400 1300 1050	490 450 410
2	3350 3200	1540	1245	1630	1360	--	1360 1300 1030	480 450
3	3390 3340 3260	1500	1200	1610	--	1650 1400	1320 1150	490 400
4	3390 3317 3200	1650	1240	1480	--	--	1330 1080	495 470 400
5	3319 3280	1520	1250	1610	1360	--	1400 1040	480 440 410
6	3450 3200 3100	1490	1200	1645	--	1490	1400 1100	490 450
7	3310 3250	1620	1240	1490	--	--	1400 1310 1050	480 450 405
8	3330 3260	1490	1250	1600	1350	--	1490 1400 1350	490 480 415
9	3430 3250	1550	1100	1610	--	1405 1650	1330 1050	490 430 405

The methods employed provide the following proposed formulas for the complexes

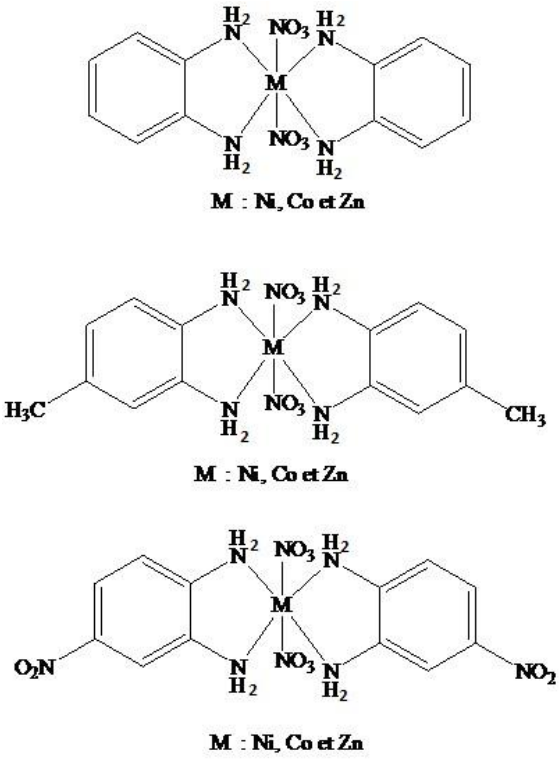

Figure 1. Chemical structures of the synthesized complexes

In Silico Analysis

Drug development faces challenges in determining the toxicity and pharmacokinetic profiles of newly synthesized compounds, as experimental evaluations are costly and time-consuming. Computational tools, such as the **admetSAR** server, have emerged as effective solutions for predicting these properties, saving significant time and resources. Cobalt's biological significance, particularly as a component of vitamin B12, makes it a valuable element in drug design. Cobalt-based complexes exhibit antimicrobial, anticancer, and anti-inflammatory activities, making them promising candidates for therapeutic applications (Cheng, 2012).

Phenylenediamine derivatives, known for their ability to coordinate with metal ions, show potential as metallo-drugs. These compounds have demonstrated effectiveness in targeting metal-dependent enzymes related to cancer, bacterial infections, and neurodegenerative diseases. They also possess significant antimicrobial, antioxidant, and biosensor applications, offering opportunities for novel therapeutic agents, diagnostics, and the treatment of oxidative stress-related diseases(wang, 2015).

This part of the study examines the pharmacokinetic and toxicological profiles of ortho-phenylenediamine (OPD), 4-methyl-ortho-phenylenediamine (MOPD), 4-nitro-ortho-phenylenediamine (Nitro-OPD), and their respective cobalt complexes (Co-OPD, Co-MOPD, Co-Nitro-OPD). Understanding these properties is crucial for assessing their potential applications in medicinal chemistry.

Absorption

- Blood–Brain Barrier (BBB) Permeability

All Free Ligands (OPD, MOPD, Nitro-OPD) are predicted to cross the blood–brain barrier with high scores (≈0.83–0.86). The unsubstituted OPD shows the highest value, whereas both substituted derivatives show a modest reduction in permeability. Complexation generally lowers the BBB permeability scores, as for OPD and MOPD (down to ≈0.66–0.76). Interestingly, the nitro-substituted complex (Co-Nitro-OPD) maintains a relatively higher value (~0.84), suggesting that the nitro group may help improve BBB penetration upon coordination with cobalt.

- Human Intestinal Absorption (HIA)

The substituted ligands, particularly Nitro-OPD (0.9228) and MOPD (0.8997), show improved predicted intestinal absorption relative to unsubstituted OPD (0.8362). The electron-withdrawing nitro group appears to favor absorption, perhaps by affecting solubility or passive diffusion properties.

All cobalt complexes show a drop in HIA scores (ranging from 0.5830 to 0.7096), indicating that complexation reduces absorption. Among these, Co-MOPD fares slightly better, suggesting that the 4-methyl substitution may mitigate the absorption-reducing effects of complexation better than the nitro group in this context.

- Caco-2 Permeability

In a model of intestinal epithelial permeability, OPD (0.7640) and MOPD (0.7364) perform better than Nitro-OPD (0.5767). This suggests that while the nitro group might improve overall intestinal absorption (as seen in HIA), it may reduce the compound’s passive permeability across cell monolayers. After complexation, the Caco-2 permeability values become quite similar (≈0.5675–0.5801) for all three derivatives. This convergence indicates that metal complexation may level the differences brought about by the substitutions.

- P-Glycoprotein (P-gp) Interaction

P-gp Substrate Profile: The probabilities for being non-substrates are moderate (≈0.66–0.78). Nitro-OPD has the highest non-substrate score (0.7763), implying it might be less likely to be expelled by P-gp pumps, potentially favoring brain penetration or retention in cells. Upon complexation, the scores drop further (≈0.5410–0.5448) for all derivatives. This indicates that cobalt complexes might be more prone to P-gp mediated efflux, though all compounds remain classified as non-substrates.

P-gp Inhibitor Profile: All free compounds have high probabilities (≈0.9216 - 0.9624) of being non-inhibitors of P-gp. Here, Nitro-OPD shows the lowest non-inhibitor probability among the free ligand.

In the complexes, the scores decrease (≈0.8306–0.8789), suggesting a somewhat higher chance of inhibiting P-gp. This could potentially affect drug-drug interactions or the distribution of co-administered substrates. All free ligands are predicted to be non-inhibitors of the renal organic cation transporter, with very similar high probabilities (≈0.903–0.9138). The complexes show slightly higher probabilities for being non-inhibitors (≈0.9085–0.9264) for OPD and MOPD. In the case of the nitro derivative, the change is minimal. Overall, substitution or complexation has only a modest effect here.

Table 3. Predicted physicochemical and pharmacokinetic properties of the studied compounds.

Property	**Model**	**OPD**	**MOPD**	**Nitro-OPD**	**Co-OPD**	**Co-MOPD**	**Co-Nitro-OPD**
ABSORPTION							
BBB Permeability	BBB+	0.8593	0.8398	0.8313	0.7564	0.6656	0.8418
HIA	HIA+	0.8362	0.8997	0.9228	0.5830	0.7096	0.6225
Caco-2 Permeability	Caco2+	0.7640	0.7364	0.5767	0.5801	0.5780	0.5675
P-gp Substrate	Non-substrate	0.7320	0.6611	0.7763	0.5410	0.5413	0.5448
P-gp Inhibitor	Non-inhibitor	0.9624	0.9529	0.9216	0.8789	0.8518	0.8306
Renal OCT Inhibition	Non-inhibitor	0.9030	0.9095	0.9138	0.9210	0.9264	0.9085
METABOLISM							
CYP450 2C9 Substrate	Non-substrate	0.8882	0.8478	0.8777	0.8247	0.7664	0.8192
CYP450 2D6 Substrate	Non-substrate	0.8921	0.8730	0.8409	0.8201	0.8230	0.8203
CYP450 3A4 Substrate	Non-substrate	0.8371	0.8139	0.6678	0.6027	0.5789	0.5806
CYP450 1A2 Inhibitor	Non-inhibitor	0.5545	0.5830	0.7257	0.5485	0.5249	0.5266
CYP450 2C9 Inhibitor	Non-inhibitor	0.6038	0.7843	0.7517	0.6587	0.6131	0.6719
CYP450 2D6 Inhibitor	Non-inhibitor	0.9762	0.9771	0.9103	0.8813	0.8810	0.8627
CYP450 2C19 Inhibitor	Non-inhibitor	0.7850	0.8626	0.5443	0.7450	0.7164	0.6780
CYP450 3A4 Inhibitor	Non-inhibitor	0.9391	0.9156	0.8566	0.7957	0.7350	0.6589
CYP Inhibitory Promiscuity	Low Inhibitory Promiscuity	0.5833	0.6004	0.6570	0.8491	0.7868	0.7532
TOXICITY							
hERG Inhibition	Weak inhibitor	0.9687	0.9640	0.8599	0.9295	0.9197	0.7343
AMES Toxicity	AMES toxic	0.9382	0.9467	0.9254	0.6234	0.6427	0.6840
Carcinogenicity	Carcinogens	0.5122	0.5208	0.5216	0.7457	0.7223	0.7594
Fish Toxicity (pLC50, mg/L)	High FHMT	1.8278	2.2131	2.1842	1.2805	1.2287	1.2263
T. pyriformis Toxicity (pIGC50, ug/L)	High TPT	0.1177	0.3287	0.4237	0.6613	0.7353	0.9624
Honey Bee Toxicity	Low HBT	0.7824	0.7992	0.7753	0.7054	0.7150	0.7124
Biodegradation	Not readily biodegradable	0.9527	0.9685	0.9826	0.9863	0.9920	0.9974
Acute Oral Toxicity	III	0.6456	0.7573	0.7152	0.5842	0.5847	0.5850
Rat Acute Toxicity (LD50, mol/kg)		2.3930	2.6245	2.5294	2.5426	2.5638	2.5499

Metabolic Stability and Enzyme Interactions

All compounds are predicted as non-substrates for major CYP450 enzymes, reducing the risk of drug-drug interactions. However, cobalt complexes exhibit higher CYP inhibitory promiscuity, indicating broader but weaker interactions with these enzymes.

Toxicity Profiling and Environmental Impact

Mutagenicity and Carcinogenicity: Non-complexed compounds show high AMES toxicity, while cobalt coordination reduces this risk by ~30% (Co-OPD = 0.6234, Co-MOPD = 0.6427), aligning with studies showing metal complexes' ability to stabilize DNA adducts and reduce reactive metabolite formation. However, cobalt complexes display elevated carcinogenicity (Yang, 2019)

Ecotoxicity: All compounds pose significant environmental risks, with cobalt complexes being extremely toxic to fish and Tetrahymena pyriformis. (Co-OPD pLC50 = 1.2805 mg/L vs. OPD = 2.3930 mg/L). Tetrahymena pyriformis: Co-Nitro-OPD (0.9624 µg/L) is 8× more toxic than Nitro-OPD (0.4237 µg/L). None of the complexes are readily biodegradable, (scores > 0.95), indicating persistence in aquatic ecosystems.

Conclusion

We report here the synthesis and spectral characterization of a series of metal complexes. Elemental analysis, IR, and UV-Vis spectroscopy confirm the successful coordination of the ligands to the metal centers, primarily through the amine groups, and indicate that the synthesized cobalt(II), nickel(II), and zinc(II) complexes adopt an octahedral geometry. The *in silico* analysis showed that free ligands (OPD, MOPD, Nitro-OPD) exhibit good absorption but high toxicity, while cobalt complexation reduces mutagenicity at the cost of lower absorption and increased environmental toxicity. All compounds are metabolically stable, but cobalt complexes show broader enzyme interactions. Thus, despite their potential in medicinal chemistry, experimental evaluation remains essential.

Scientific Ethics Declaration

* The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM Journal belongs to the authors.

Conflict of Interest

* The authors declare that they have no conflicts of interest

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