

Research Article:

Ni(II) Metal Complexes with 1-Phenylsemicarbazide and Phosphine Ligands: Synthesis, Characterization and Computational Studies

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Abstract

Background: In coordination chemistry, the derivatives of semicarbazide ligand are more attractive ligands due to variable coordination mode as well as its capacity to synthesize stable complexes via its nitrogen and carbonyl oxygen donor atoms.

Aims: This study describes the synthesis, characterization, biological evaluation, and computational calculation of a new series Ni(II) mixed-ligand complexes involving 1-phenylsemicarbazide (PSC) and some tertiary phosphine ligands.

Methodology: A one-pot synthetic approach was used for the synthesis of a series of five Ni(II) complexes, [NiCl(PSC)(PPh₃)] (1), [Ni(PSC)(dppm)]Cl (2), [Ni(PSC)(dppe)]Cl (3), [Ni(PSC)(dppp)]Cl (4), and [Ni(PSC)(dppf)]Cl (5). The complexes were characterized by FT-IR, ¹H and ³¹P{¹H} NMR, UV–Vis spectroscopy, CHN elemental analysis, magnetic susceptibility, and molar conductivity measurements. Antibacterial properties of the complexes were examined against Gram-positive *Staphylococcus aureus* and Gram-negative *Escherichia coli*. Density functional theory (DFT), natural bond orbital (NBO), and molecular electrostatic potential (MEP) studies were employed to elucidate electronic properties and chemical reactivity.

Results: Spectroscopic and physicochemical characterization suggests a square-planar geometry of all the synthesized Ni(II) coordination compounds. Computational studies revealed that complex 4 displayed better stability and lower reactivity, however complex 1 exhibited higher reactivity and lower stability. Antibacterial results established that complex 3 displayed the greatest antibacterial activity toward both bacterial strains.

Conclusion: Successful synthesis and characterization of several new mixed-ligand Ni(II) complexes involving PSC and some tertiary phosphine ligands was achieved. A distorted square-planar geometry for the complexes was suggested as a result of the characterization data and computational investigations, which also suggested possible structure–stability–activity relationships pertinent to future biological investigations.

Keywords: Computational Studies, Antibacterial activity, Ni(II) complexes, 1-Phenyl semicarbazide, Phosphines.

1. Introduction

Semicarbazide and its compounds, due to the excellent coordination property and high stability of the complexation tendency, have been recognized as important ligands in coordination chemistry [1]. These ligands demonstrate highly flexible coordination behavior, with the coordinating nitro-

gen and oxygen donor sites enabling them to act as bidentate or tridentate chelating ligands depending on structural features [2]. As a result, ligands based on semicarbazide can coordinate to metal ions in different coordination geometries of complex ones like square-planar, tetrahedral or octahedral [3,4]. Apart from their structural diversity, derivatives of semicarbazide and their coordination compounds have received considerable attention owing to a wide range

of biological activities including antimicrobial, antifungal, anticancer, antiviral and anti-inflammatory effects [5,6]. Due to these properties, they can be considered as promising components for potential biomedical applications of functionally coordinative compounds. Similarly, nickel (II) mixed-ligand complexes (especially those containing nitrogen- and phosphorus-donor ligands) have been the subject of much research due to their coordination versatility, adjustable electronic properties, and relevance in catalysis and bioinorganic chemistry [7]. These studies demonstrate that tertiary phosphine ligands greatly influence the electronic properties and stability of metal centers, often causing discrete geometries and enhanced reactivity. However, although a variety of semicarbazide ligands and nickel complexes containing tertiary phosphine have been studied, mixed-ligand nickel (II) complexes with the combination of 1-phenylsemicarbazide (PSCH) and tertiary phosphine have not yet been reported. This is a clear indication of the gap within coordination chemistry in semicarbazide systems. In this context, a new family of nickel (II) mixed-ligand complexes containing PSC^- and tertiary phosphine ligands. Their antibacterial activity was examined against Gram-positive *Staphylococcus aureus* (*S. aureus*) and Gram-negative *Escherichia coli* (*E. coli*). In addition, DFT, NBO and MEP analysis were also carried out to gain more insight into their electronic structure, stability and reactivity.

2. Experimental

2.1. Material and Methods

All chemicals, including $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, PSCH, PPh_3 , dppm, dppe, dppp, and dppf, were Purchased from Sigma-Aldrich and used without further purification. Solvents such as ethanol ($\text{CH}_3\text{CH}_2\text{OH}$, 99.9%), dichloromethane (99.8%), and dimethyl sulfoxide (DMSO, 99.8%) were obtained from Sharlau and used as received.

Infrared spectra were recorded on a Shimadzu IR Affinity spectrophotometer (CORPA21375003225) over the $400\text{--}4000\text{cm}^{-1}$ range using potassium bromide (KBr) pellet technique. $^{31}\text{P}\{^1\text{H}\}$ and ^1H NMR spectra were acquired on a Bruker Avance 400 MHz spectrometer (^{31}P : 161.9 MHz, ^1H : 400 MHz) in $\text{DMSO}-d_6$ as the solvent. CHN elemental analyses were performed using a Thermo Fisher EA 300 analyzer. Magnetic susceptibility measurements were carried out using a Sherwood Scientific Magnetic Susceptibility Balance (MSB Mk1, UK). UV–Vis electronic spectra were recorded on a Shimadzu UV-1900i spectrophotometer in DMSO (1×10^{-3} M) over the 200–800 nm range using quartz cuvettes. Molar conductivity measurements were conducted in DMSO (1×10^{-3} M) at 25°C using a Jenway 4520 conductivity meter. Melting points were determined using an MPD-100 melting point apparatus (Pixel Technology Co., Ltd.).

2.2. Synthesis of $[\text{NiCl}(\text{PSC})(\text{PPh}_3)]$ Complex 1

A warm ethanolic solution of KOH (0.6 mmol, 0.0336 g in 5 mL ethanol) was added to a warm ethanolic solution of PSCH ligand (0.6 mmol, 0.0907 g in 5 mL ethanol) and

stirred at room temperature for 1 h. The resulting clear solution was then added dropwise to an ethanolic solution (5 mL) of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (0.6 mmol, 0.1425 g), and the reaction mixture was refluxed at 50°C for 3 h. During this period, the solution color changed from pale green to dark orange, indicating the formation of the complex. Subsequently, an ethanolic solution of triphenylphosphine (PPh_3) (1.2 mmol, 0.314 g) was added, and the mixture was further refluxed for an additional 2 h. The resulting orange solution was then filtered to remove any insoluble impurities, and the filtrate was left to evaporate slowly at room temperature. The resulting orange solid was collected by filtration, washed, and dried in air. Yield: 1.075 g (82%), m.p. $100\text{--}103^\circ\text{C}$.

The complexes: Complex 2: $[\text{Ni}(\text{PSC})(\text{dppm})]\text{Cl}$, Complex 3: $[\text{Ni}(\text{PSC})(\text{dppe})]\text{Cl}$, Complex 4: $[\text{Ni}(\text{PSC})(\text{dppp})]\text{Cl}$, and Complex 5: $[\text{Ni}(\text{PSC})(\text{dppf})]\text{Cl}$ were synthesized and isolated using the same procedure, except that dichloromethane was used as the solvent for dissolving the respective phosphine ligands instead of ethanol.

2.3. Antimicrobial Activity

The bacterial strains *S. aureus* and *E. coli* were obtained from the Microbiology Laboratory of the College of Science, Department of Biology, Salahaddin University. The bacterial isolates were obtained from clinical specimens collected at Rezgari Hospital at Rezgari hospital.

E. coli isolated from UTI infections and *S. aureus* isolated from wound infection. The isolates were classified as multidrug-resistant (MDR), the isolated bacteria are MDR. It means they were resistant to at least three antimicrobial classes of antibiotics.

The strains were maintained as stock cultures under standard laboratory conditions and used throughout the antibacterial assays. Identification was previously confirmed in the laboratory using conventional microbiological techniques, including Gram staining, colony morphology, and standard biochemical tests. No molecular or automated identification methods were employed. The strains were utilized as laboratory reference cultures for preliminary antibacterial screening, and no detailed antimicrobial susceptibility profiles were available for the tested organisms.

The antibacterial activity of the synthesized nickel (II) complexes 1–5 was assessed against *S. aureus* and *E. coli* using a modified agar disk diffusion method in accordance with the Clinical and Laboratory Standards Institute (CLSI) guidelines for antimicrobial susceptibility testing (CLSI document M100, 30th edition, 2020).

Muller–Hinton agar (20 mL) was poured into sterile Petri dishes and allowed to solidify. Bacterial inocula were prepared in nutrient broth and adjusted to a final concentration of about 1.5×10^8 CFU/mL (0.5 McFarland standard) (McFarland, 1907) [28]. For the determination of antimicrobial activity, 100 μL of the standardized inoculum was spread evenly over the surface of an agar plate using a sterile swab to produce a confluent lawn of growth. For preparing the synthesized complexes as solid forms, a disk consisting of 1:4 (mg per disk) KBr and solid complex was compressed to provide similar dosing and mechanical stability. Disks were placed on the agar surface 15 min after

inoculation. Plates incubated at 37 °C for 24 h were used to evaluate the antibacterial activity by measuring the diameter of each inhibition zones (mm) around. To compare under similar conditions, standard antibiotics (Vancomycin and Meropenem) were also used. It should be noted that KBr was employed only as an inert matrix for disk preparation and is not a standard biological solvent, which represents a limitation of the experimental design. No inhibition was observed for the KBr control disks under the applied conditions. In addition, the absence of inhibition zones for the reference antibiotics Vancomycin and Meropenem was unexpected and constitutes an additional limitation of the present study. Since no additional validation experiments were performed, these findings should be interpreted with caution, as factors related to the experimental conditions may have influenced the observed results. Calculation of mean $\pm$ SD was not possible because only a single measurement was obtained.

2.4. Computational Details

Gaussian 09 software was employed to carry out theoretical calculations on the ligands and their corresponding Ni(II) complexes, including DFT, NBO, and MEP analyses. Geometry optimizations of the ligands were performed using the B3LYP hybrid functional with the 6-31G(d) basis set, whereas the nickel (II) complexes were optimized using the B3LYP functional together with the LANL2DZ for the metal center. Complex 5 was excluded from the DFT calculations because it contains a ferrocene (dppf) fragment with

an iron center, which introduces additional spin-state complexity that lies beyond the scope of the present investigation.

3. Result and Discussion

3.1. Synthesis and Characterization of Complexes

Treatment of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ with equimolar amounts of PSCH and tertiary phosphine ligands afforded mixed-ligand complexes of the type $[\text{NiCl}(\text{PSC})(\text{PPh}_3)]$ complex 1 and $[\text{Ni}(\text{PSC})(\text{diphos})]\text{Cl}$, where diphos = dpmm complex 2, dppe complex 3, dppp complex 4, or dppf complex 5. Complex 1 was obtained in ethanol, whereas complexes 2–5 were synthesized in a mixed ethanol–dichloromethane solvent system, with yields ranging from 68–87% (Figure 1). The synthesized complexes were characterized by FT-IR, $^{31}\text{P}\{^1\text{H}\}$ and ^1H NMR spectroscopy, elemental analysis, magnetic susceptibility measurements, electronic spectroscopy, and molar conductivity measurements. All complexes are proposed to exhibit square-planar geometry based on the available characterization data.

To the best of our knowledge, no directly related mixed-ligand Ni(II) complexes containing both PSCH and phosphine ligands have been reported. Nevertheless, the obtained spectroscopic and structural features are generally consistent with previously reported Ni(II)-phosphine complexes and semicarbazide-derived nickel complexes. The coordination behavior of the ligand was confirmed by FT-IR, NMR, and electronic spectral analyses.

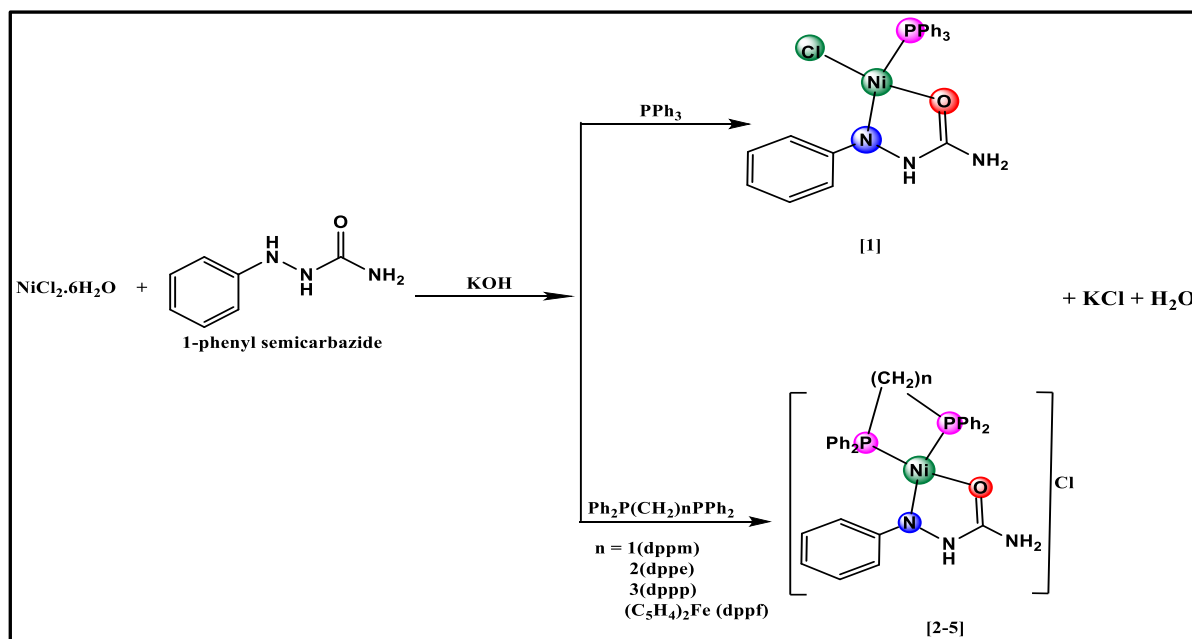


Figure 1: Proposed synthetic pathway for the preparation of Ni(II) mixed-ligand complexes (1–5) containing (PSC[−]) and tertiary phosphine ligands.

3.2. Elemental Analysis

Table 1 summarizes the CHN elemental analysis together with the physical and chemical properties of the synthesized complexes. The Ni(II) complexes were prepared from Ni(II) salts in the presence of PSCH and various aromatic phosphine ligands. The syntheses were carried out in a 1:1 metal-to-ligand molar ratio. The carbon and nitrogen elemental analysis results for complex 1 are less than 0.5% different from the expected results. They are consistent with the proposed composition. According to the test results for complex 2, the nitrogen and carbon values are within 0.15% of the predicted values. These findings indicate that the sample is quite clean, but elemental analysis results for complex 3 depart somewhat from the calculated results; the quantities of carbon and nitrogen are lower by 0.68% and

0.58%, respectively. These discrepancies are somewhat greater than ideal. However, the complex 4 test results indicate that the differences are less than 0.4% of the expected values. This confirms the proposed formula, demonstrates the purity of the isolated chemical. Finally, the most variable was observed in complex 5 especially in the carbon content, which is roughly 1.23% lower than expected because of the compound's partial disintegration during storage or analysis residual moisture or retained solvent molecules, and the sample's partial dryness during analysis are the reasons for these variances and these ranges are suitable for coordination compounds.

This is consistent with the proposed molecular formulas. Elemental analysis data support the formation of the complexes and indicate the coordination of one deprotonated PSCH ligand together with one mole of the co-ligand (aromatic phosphine).

Table 1: Physical properties and CHN elemental analysis of the synthesized Ni(II) complexes (1–5).

Complex No.	Chemical formula & M.Wt(g/mol)	Colour	Yield %	M.P (°C)	Calcd. (Found)		
					% C	% H	% N
1	C ₂₅ H ₂₃ N ₃ POCINi 506.59	Orange	82	100-103	59.26 (58.90)	4.57 (4.77)	8.29 (7.80)
2	C ₃₂ H ₃₀ N ₃ P ₂ OCINi 628.69	Red	68	177-179	61.13 (61.26)	4.81 (4.37)	6.67 (6.59)
3	C ₃₃ H ₃₂ N ₃ P ₂ OCINi 642.72	Orange	87	299-302	61.66 (60.98)	5.01 (4.97)	6.53 (5.95)
4	C ₃₄ H ₃₄ N ₃ P ₂ OCINi 656.74	Brown	81	113-116	62.17 (61.87)	5.21 (5.14)	6.39 (6.03)
5	C ₄₁ H ₃₆ N ₃ P ₂ OFcCINi 798.68	Orange	77	176*	61.65 (60.42)	4.54 (4.91)	5.25 (4.96)

* = decomposition

3.3. FT-IR Spectroscopy

The FT-IR spectra of complexes 1–5 (Figures 2–4, Table 2) show absorption bands in the 3479–3414 cm⁻¹ region is assigned to the ν (NH₂) stretching vibrations of the PSC⁻ ligand, suggesting that the amino group remains unaltered upon coordination [5]. Bands appearing in the 3267–3234 cm⁻¹ region are attributed to the ν (NH) stretching vibrations of the semicarbazide fragment. However, the existence of these absorptions does not exclude the possibility of deprotonation at other positions within the ligand structure. The ν (C=O) absorption of the PSC⁻ ligand, observed at 1691–1639 cm⁻¹, is shifted to lower wavenumbers relative to the free ligand, indicating coordination of the carbonyl oxygen atom to the Ni(II) center [8]. In addition, the phosphine ligands exhibit characteristic absorption bands at 1431–1436

cm⁻¹ and 540–570 cm⁻¹ is assigned to ν (P–Ph) and ν (P–C) stretching vibrations, respectively [9]. The FT-IR spectra of complexes 1–5 further show new bands in the 534–570 cm⁻¹ and 451–474 cm⁻¹ regions, attributable to ν (Ni–O) and ν (Ni–N) vibrations, respectively, thereby confirming coordination through oxygen and nitrogen donor atoms [6,8]. The ν (NH₂) bands in the spectra indicate that the amino group is still protonated, but it cannot confirm deprotonation of –NH–Ph just with FT-IR spectroscopy. However, if considered in combination with the ¹H NMR data, these findings are consistent with a largely selective deprotonation at the –NH–Ph site to yield a monoanionic coordination mode of the PSC⁻ ligand.

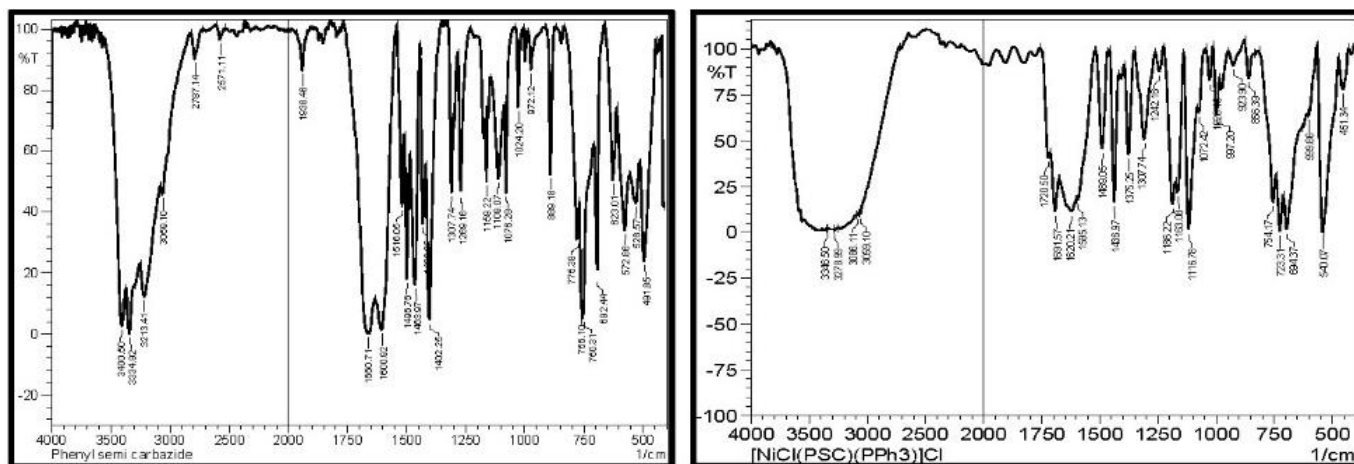


Figure 2: FT-IR spectra of the free PSCH ligand and complex 1, [NiCl(PSCH)(PPh₃)].

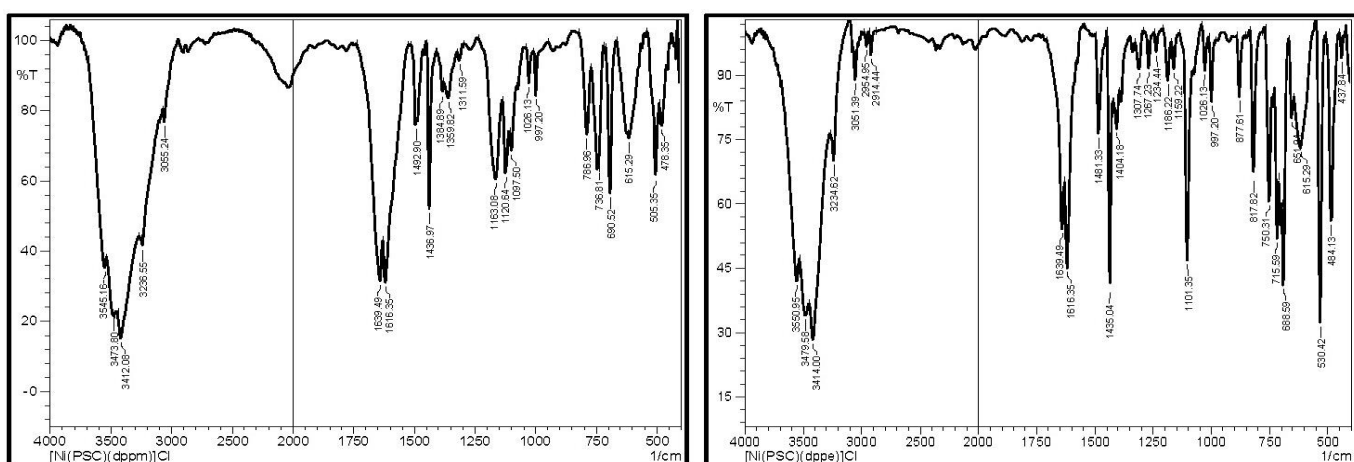


Figure 3: Comparative FT-IR spectra of Ni(II) complex 2, [Ni(PSCH)(dppm)]Cl and complex 3, [Ni(PSCH)(dppe)]Cl.

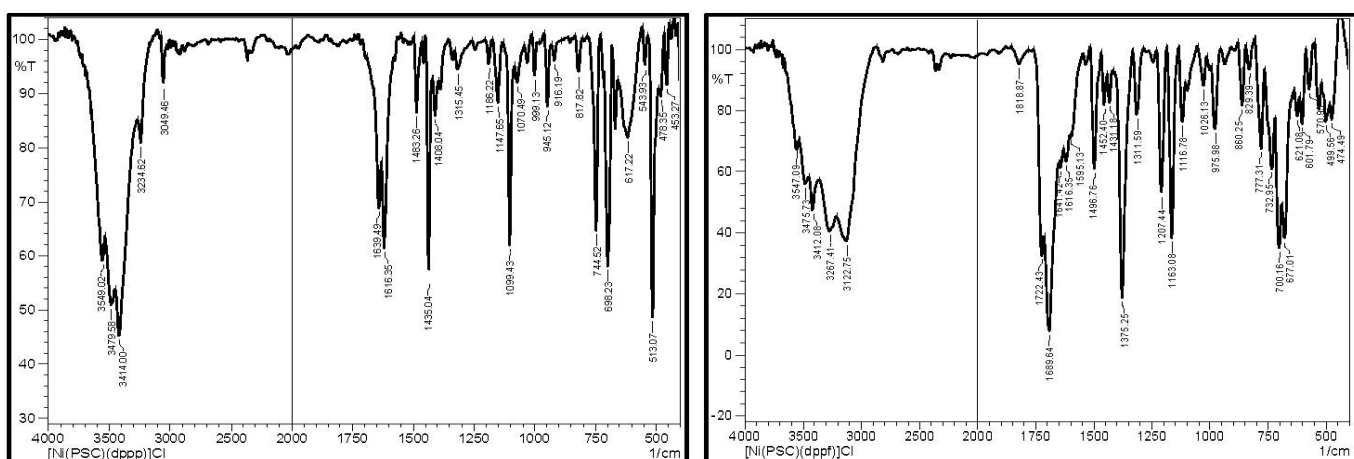


Figure 4: FT-IR spectra of complex 4, [Ni(PSCH)(dppp)]Cl, and complex 5, [Ni(PSCH)(dppf)]Cl.

Table 2: Characteristic FT-IR absorption bands (cm^{-1}) of the free PSCH ligand and Ni(II) complexes (1–5)

Complexes	NH ₂	N-H	C-H arom.	C-H alph.	C=O	P-Ph	P-C	M-O	M-N
PSCH	3400, 3334	3213	3059	2787	1660	...	...	...	...
1	3345-3330	3276	3096		1691	1436	694	540	451
2	3473-3414	3236	3055	2899	1639	1436	690	505	478
3	3479-3414	3234	3051	2914	1639	1435	688	530	484
4	3479-3412	3234	3049	2827	1639	1435	698	513	453
5	3475-3412	2367	3056		1689	1475	677	570	488

3.4. $^{31}\text{P}\{^1\text{H}\}$ NMR Spectroscopy

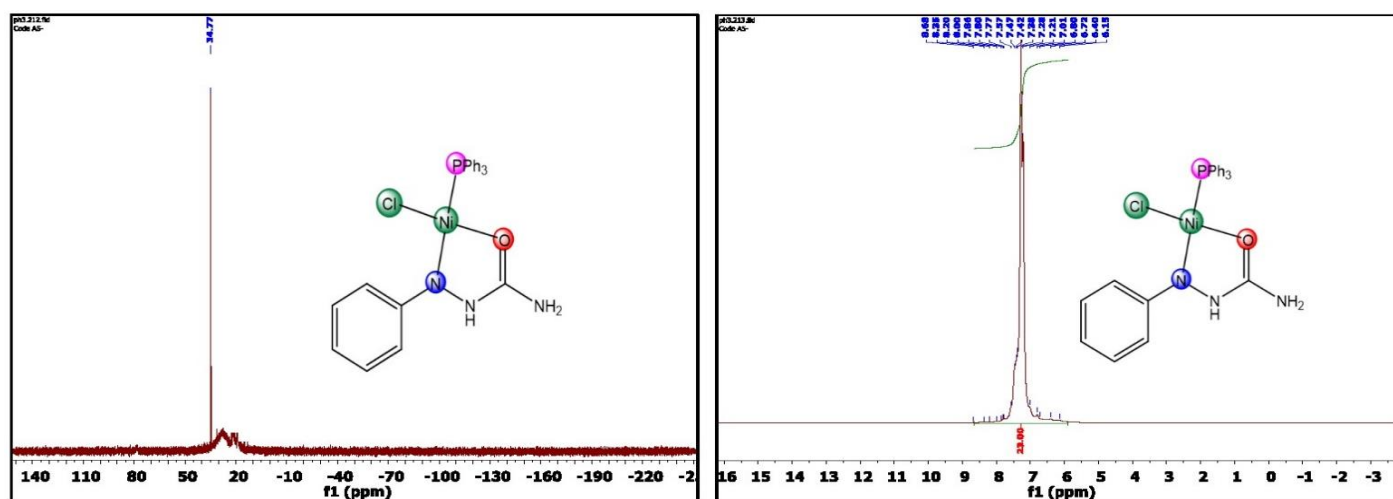
The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex 1 (Fig. 5, Table 3) displays a singlet at $\delta\text{P} = 34.77$ ppm. Only a single resonance is observed to indicate the presence of a similar phosphine environment, which is consistent with PPh_3 coordination on the opposite side of the nitrogen donor atom of PSC- ligand, signifying trans complex structure [10,11].

The spectra of 2–5 (Figures 6–9) each show two overlapping resonances, indicative of somewhat broadened doublets characteristic for an AX spin system that fit to We see these doubly peaked phosphorus signals due to the presence of two magnetically inequivalent phosphorus nuclei [10,12]. The observed chemical shifts are $\delta\text{PA} = 36.21$ ppm and $\delta\text{PX} = 21.08$ ppm for complex 2 ($2J(\text{PA-PX}) = 3$ Hz.), $\delta\text{PA} = 58.83$ ppm and $\delta\text{PX} = 30.22$ ppm for complex 3 ($2J(\text{PA-PX}) = 47$ Hz), $\delta\text{PA} = 30.57$ ppm and $\delta\text{PX} = 22.78$ ppm for complex 4 ($2J(\text{PA-PX}) = 2$ Hz), and $\delta\text{PA} = 36.03$ ppm and $\delta\text{PX} = 20.17$ ppm for complex 5 ($2J(\text{PA-PX}) = 3$ Hz) [10–12]. These spectral patterns indicate that the two phosphorus atoms reside in different chemical environments: one phosphorus (PA) is trans to the carbonyl oxygen of the PSC- ligand, while the other (PX) is trans to the nitrogen donor atom. This in equivalence of the phosphorus centers supports an asymmetric coordination environment in all complexes studied [13–15].

3.5. ^1H NMR Spectroscopy

The ^1H NMR spectra of complexes 1–5 (Figures 5–9, Table 3) were recorded in DMSO- d_6 with TMS as an internal standard. The spectra show multiplet signals in the δ 9.34–4.72 ppm region, corresponding to the aromatic protons of both the PSC- and phosphine ligands. In addition, resonance is assigned to the NH_2 protons of the PSC- ligand are observed in most complexes, indicating that this group remains protonated after coordination [16–20]. In the free PSCH ligand, the $-\text{NH}-\text{Ph}$ proton is observed as a singlet at δ 9.55 ppm. This resonance is not detected in the ^1H NMR spectra of complexes 1–5, indicating that deprotonation of this NH group occurs upon coordination to the Ni(II) center.

This disappearance supports the participation of the deprotonated nitrogen atom in metal binding. The aliphatic proton signals of the dppe, dppe, and dppp ligands in complexes 2–4 appear in the δ 0.73–2.34 ppm range as triplet, singlet, and multiplet resonances, respectively. For complex 5, the cyclopentadienyl (Cp) protons of the dppf ligand are observed as multiplets between δ 0.37–4.46 ppm [21]. The ^1H NMR data suggest that the PSC- ligand undergoes selective deprotonation at the $-\text{NH}-\text{Ph}$ site, while the NH_2 group remains protonated, leading to a monoanionic coordination mode. This interpretation is in good agreement with the FT-IR result.

**Figure 5:** $^{31}\text{P}\{^1\text{H}\}$ and ^1H NMR spectra of complex 1 $[\text{NiCl}(\text{PSC})(\text{PPh}_3)]$

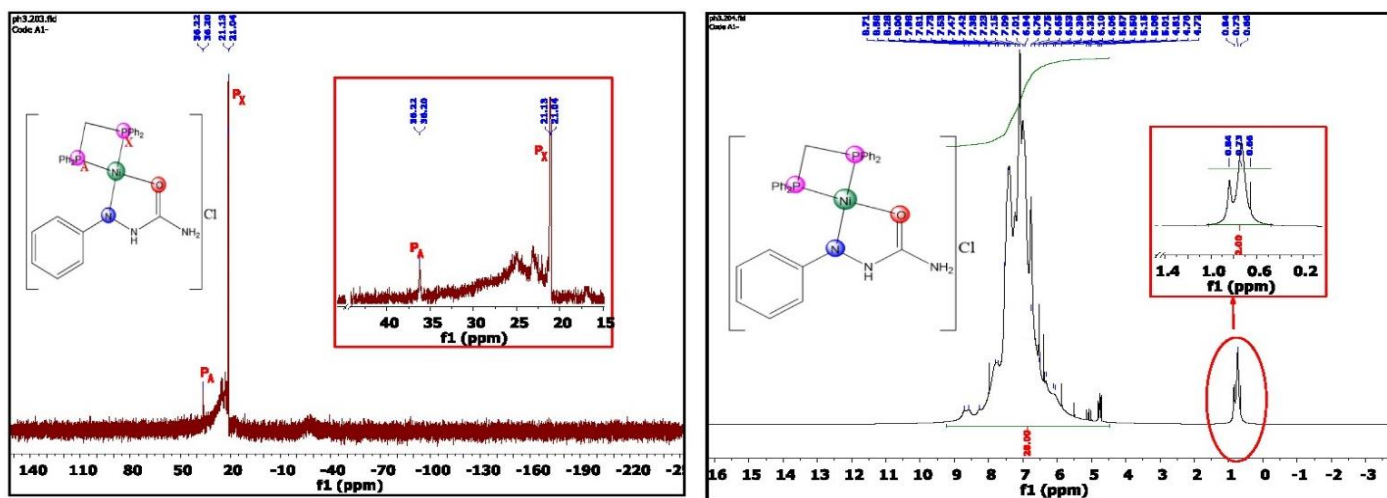


Figure 6: ^{31}P -{ ^1H } and ^1H NMR spectra of complex 2, $[\text{Ni}(\text{PSC})(\text{dppm})]\text{Cl}$, including expanded views of the phosphorus resonances and methylene proton signals.

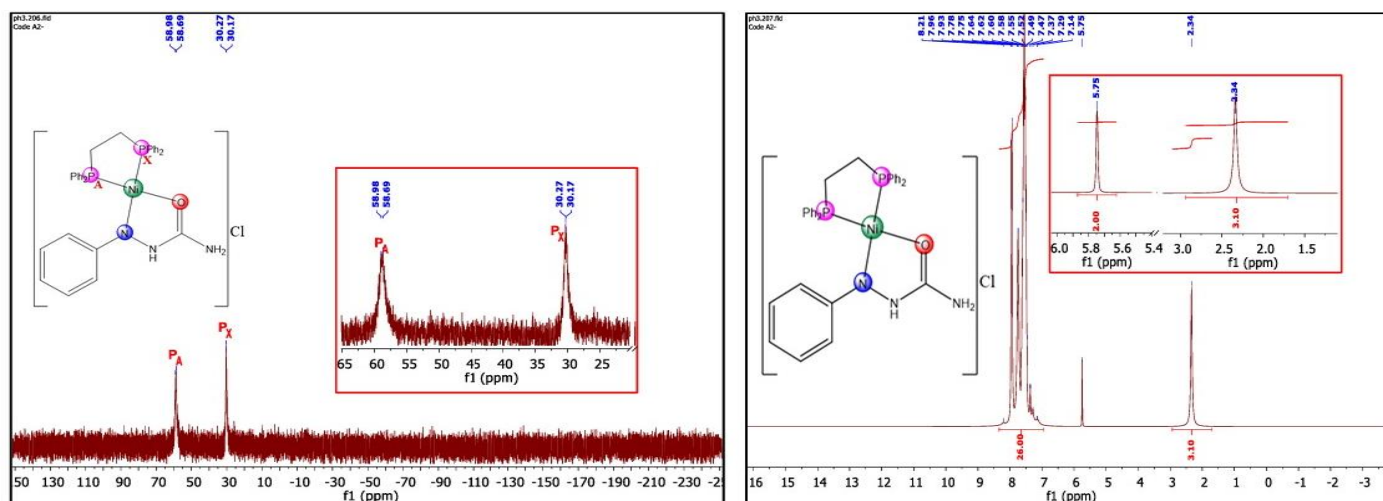


Figure 7: ^{31}P -{ ^1H } and ^1H NMR spectra of complex 3, $[\text{Ni}(\text{PSC})(\text{dppe})]\text{Cl}$, including expanded views of the phosphorus resonances and characteristic proton signals.

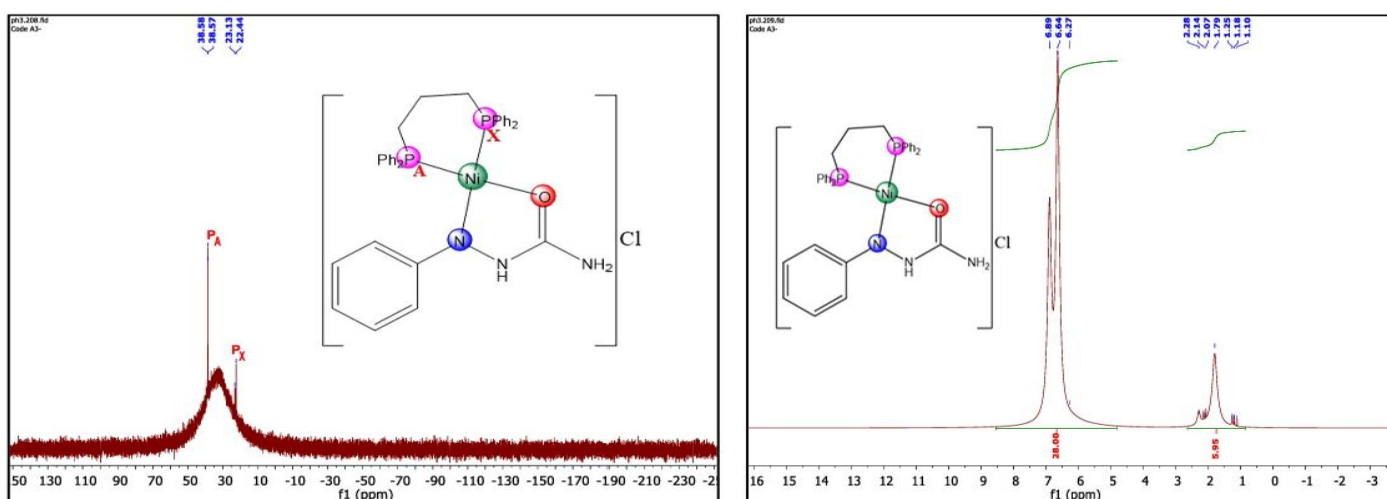
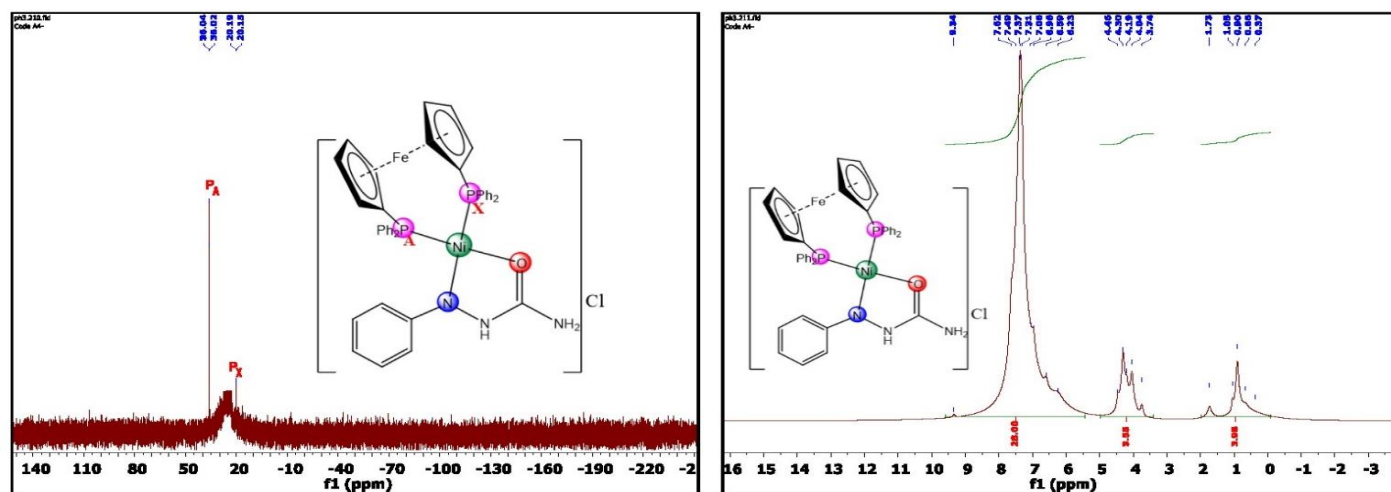


Figure 8: ^{31}P - $\{^1\text{H}\}$ and ^1H NMR spectra of complex 4, $[\text{Ni}(\text{PSC})(\text{dppp})]\text{Cl}$

Figure 9: $^{31}\text{P}\{-^1\text{H}\}$ and ^1H NMR spectra of complex 5, $[\text{Ni}(\text{PSC})(\text{dppf})]\text{Cl}$.Table 3: $^{31}\text{P}\{-^1\text{H}\}$ and ^1H NMR chemical shifts for complexes (1-5)

Complex No.	δP ppm	δH ppm
1	$\delta\text{P} = 34.77$	6.15-8.68 (m, 23H, Ph, NH, NH_2).
2	$\delta\text{P}_\text{A} = 36.22, 36.20$ ($^2\text{J}_{(\text{PA-PX})} = 3$ Hz.), $\delta\text{P}_\text{X} = 21.13, 21.04$	4.72-8.71 (m, 28H, Ph, NH, NH_2), 0.73 (t, $^3\text{J}_{(\text{H-H})} = 36$ Hz., 2H, CH_2).
3	$\delta\text{P}_\text{A} = 58.98, 58.69$ ($^2\text{J}_{(\text{PA-PX})} = 47$ Hz.), $\delta\text{P}_\text{X} = 30.27, 30.17$	7.14-8.21 (m, 26H, Ph, NH), 5.75 (s, 2H, NH_2), 2.34 (s, 4H, CH_2)
4	$\delta\text{P}_\text{A} = 38.58, 38.57$ ($^2\text{J}_{(\text{PA-PX})} = 2$ Hz.), $\delta\text{P}_\text{X} = 23.13, 22.44$	6.17-6.89 (m, 28H, Ph, NH, NH_2), 1.10-2.28 (m, 6H, CH_2).
5	$\delta\text{P}_\text{A} = 36.04, 36.02$ ($^2\text{J}_{(\text{PA-PX})} = 3$ Hz.), $\delta\text{P}_\text{X} = 20.19, 20.15$	6.23-9.34 (m, 28H, Ph, NH, NH_2), 3.74-4.46 (m, 4H, Cp), 0.37-1.73 (m, 4H, Cp).

3.6. Electronic Spectroscopy and Molar Conductivity

The ligand and its metal complexes' absorption spectra were recorded in DMSO within the 200-800 nm range. (PSC) and other phosphine ligands (PPh_3 , dppm , dppe , dppp , dppf) exhibit characteristic absorption bands associated to (PSC-) with d-d transitions, charge transfer (C.T.), and ligand field excitation in the UV-Vis spectral data of the proposed to exhibit distorted square-planar Ni(II) complexes (Figures 10 and 11 and Table 4).

Representative d8 systems with a low-spin structure and diamagnetism are proposed to exhibit square-planar Ni(II) complexes. Charge transfer interactions, (d-d) stimulation, and ligand-based $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions all affect their UV-Vis spectra. These spectrum signals are highly sensitive indicators of metal-ligand binding, analytic geometry, and ligand electronic effects. At around 255 nm, ligand-based $\pi \rightarrow \pi^*$: agrees with phosphine ligands and aromatic π orbitals seen in PSC. These bands, which correspond to intra-ligand $\pi \rightarrow \pi^*$ transitions within the PSC- section, form at around 255-256 nm for all compounds. These transitions' high energy is consistent with the usual aromatic $\pi \rightarrow \pi^*$ excitation [22,23].

Non-bonding $n \rightarrow \pi^*$ (~273 nm): attributable to lone pairs of heteroatoms, namely nitrogen, that participate in $n \rightarrow \pi^*$ transitions. These transitions, which take place between 273 and 275 nm, include the movement of non-bonding electrons on heteroatoms (like nitrogen) to π^* orbitals. These are signs of lone pairs on nitrogen atoms and other PSC ligands. Transfer of charge (C.T.) (~351-355 nm): Ligand-to-metal charge transfer is the cause of these bands.

These bands are typical in a proposed distorted square-planar Ni(II) complexes with π -acceptor ligands and suggest electron transport from ligand orbitals to the Ni(II) center [24].

Transitions from $1\text{A}_1 \rightarrow 1\text{A}_2$ and $1\text{A}_1 \rightarrow 1\text{B}_2$ are responsible for the d-d transitions (~417-662 nm). A specific transition is assigned to the bands at longer wavelengths (417, 662 nm) in complex 4 and (467, 544 nm) in complex 1. Accordingly, $1\text{A}_1 \rightarrow 1\text{A}_2$ and $1\text{A}_1 \rightarrow 1\text{B}_2$. The ligand field strength and, thus, the energy of d-d transitions are determined by the (PSC-) ligand's which exhibits a d-d transition at (544 nm), complexes containing more electron-rich or chelating phosphines, such as (dppp), have lower energy d-d bands (662 nm), indicating a weaker ligand field [25]. As is common for Ni(II) complexes with strong field ligands, all complexes have similar spectrum characteristics consistent with a proposed distorted square-planar geometry. The charge transfer bands demonstrate that the presence of PSC- and phosphines creates a ligand-supporting environment for π -acceptor interactions. The complexes are diamagnetic, which is consistent with a proposed distorted square-planar Ni(II) d8 configuration, in which every electron is paired in the ligand field. In a low-spin a proposed distorted square-planar environment, this helps assign the observed d-d transitions to ligand field excitations [26].

All complexes were measured for molar conductance utilizing a 10⁻³ molar concentration (DMSO) solution; the data, as shown in Table 4, signify that all complexes function as electrolytes except complex 1. The molar conductance values range from 32.6-37.5 $\text{cm}^2 \Omega^{-1} \text{mol}^{-1}$, which is consistent with a 1:1 electrolyte type. This conclusion is supported by positive tests with AgNO_3 for complexes con-

taining chloride ions, which confirm the presence of chloride. However, the complex 1 does not exhibit electrolyte demeanor, these findings indicate that it is non-electrolyte under test conditions [27].

3.7. Magnetic Susceptibility Measurements

Important information about the oxidation state and stereochemistry of the Ni(II) metal in coordination complexes is provided by magnetic characteristics. The magnetic susceptibility measurements of Ni+2 complexes ($\mu_{\text{eff}} \sim 0$) denotes that the synthesized compounds support the proposed distorted square-planar geometry (Table 4) [26].

Table 4: Electronic spectroscopy (UV-Vis) and molar conductivity measurements of PSCH ligand and complexes (1-5)

Complexes No.	Absorption cm^{-1}	Absorption nm.	Molar absorptivity (ϵ)	Assignment	Magnetic susceptibility μ_{eff}	$\Delta_M(\Omega^{-1}\text{cm}^2\text{mol}^{-1})$ in DMSO
PSCH	39215	255	0.351×10^3	$\pi \rightarrow \pi^*$	-----	1.25
	34722	288	0.169×10^3	$n \rightarrow \pi^*$		
	39062	256	1.187×10^3	$\pi \rightarrow \pi^*$		
	36496	274	0.914×10^3	$n \rightarrow \pi^*$		
1	28248	354	0.604×10^3	C.T	0.10	8.65
	21413	467	0.363×10^3	$^1A_1 \rightarrow ^1A_2$		
	18382	544	0.152×10^3	$^1A_1 \rightarrow ^1B_2$		
	39215	255	0.804×10^3	$\pi \rightarrow \pi^*$		
2	36630	273	0.438×10^3	$n \rightarrow \pi^*$	0.09	32.6
	28490	351	0.608×10^3	C.T		
	23584	424	0.385×10^3	$^1A_1 \rightarrow ^1A_2$		
	18761	533	0.356×10^3	$^1A_1 \rightarrow ^1B_2$		
3	39215	255	0.438×10^3	$\pi \rightarrow \pi^*$	0.11	33.4
	36496	274	0.279×10^3	$n \rightarrow \pi^*$		
	28409	352	0.204×10^3	C.T		
	22321	448	0.170×10^3	$^1A_1 \rightarrow ^1A_2$		
4	18656	536	0.089×10^3	$^1A_1 \rightarrow ^1B_2$	0.08	37.5
	39062	256	0.483×10^3	$\pi \rightarrow \pi^*$		
	36630	273	0.310×10^3	$n \rightarrow \pi^*$		
	28169	355	0.223×10^3	C.T		
5	23980	417	0.194×10^3	$^1A_1 \rightarrow ^1A_2$	0.12	34.8
	15105	662	0.103×10^3	$^1A_1 \rightarrow ^1B_2$		
	39215	255	1.956×10^3	$\pi \rightarrow \pi^*$		
	36363	275	1.066×10^3	$n \rightarrow \pi^*$		
5	28328	353	0.710×10^3	C.T	0.12	34.8
	22573	443	0.748×10^3	$^1A_1 \rightarrow ^1A_2$		
	17064	586	0.156×10^3	$^1A_1 \rightarrow ^1B_2$		

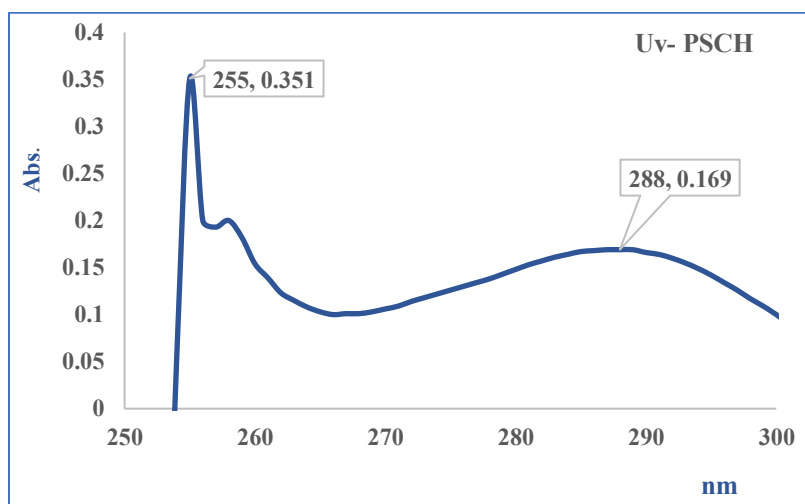


Figure 10: Uv and ($\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$) transitions spectra of PSCH ligand

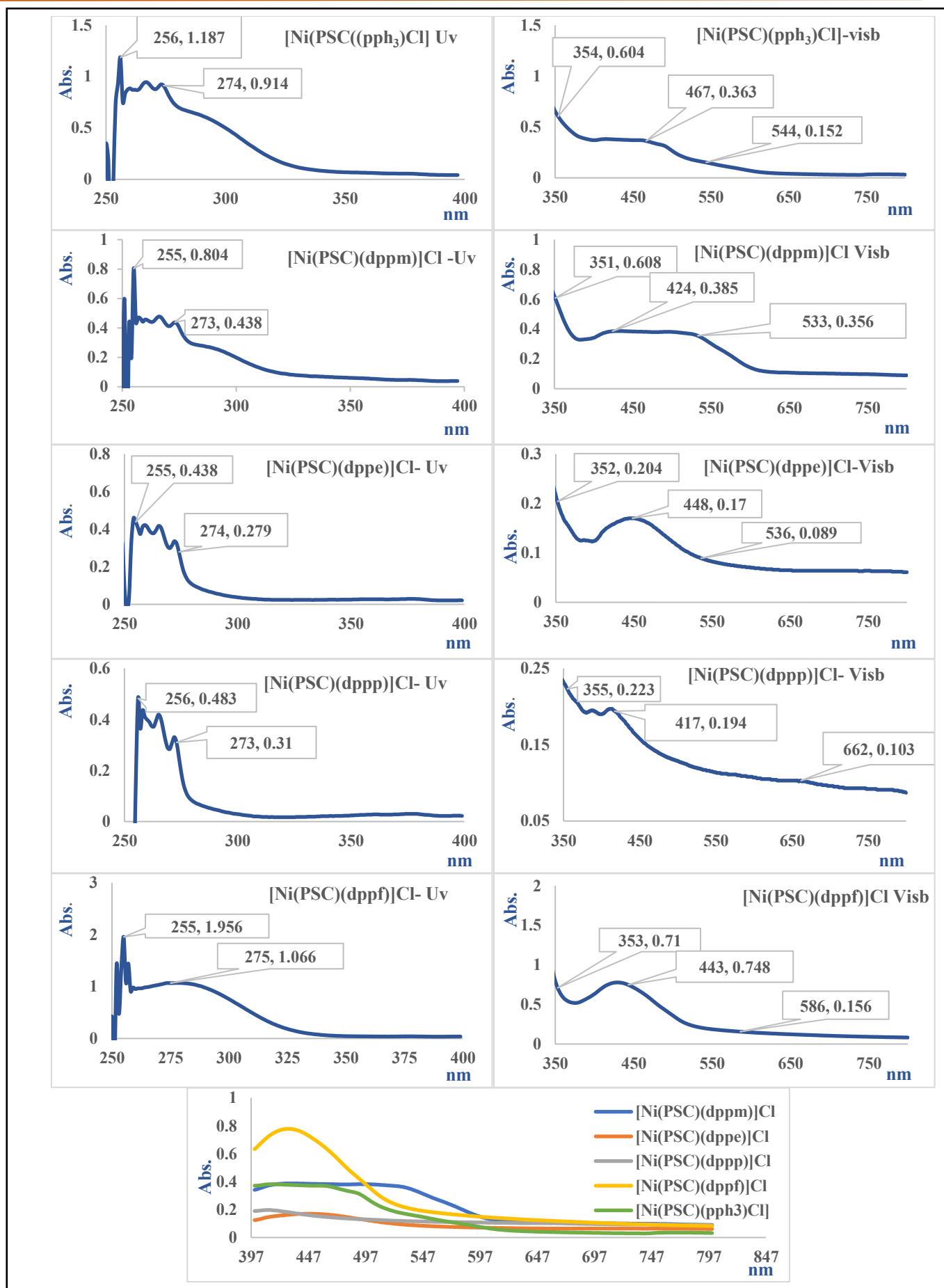


Figure 11: Electronic spectra { $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ and d-d transitions} of a proposed distorted square-planar complexes (1-5)
 {Abs.=Absorbance, nm= wave length}

3.8. Antibacterial Activity

The antibacterial activity of Ni(II) complexes 1–5 was assessed against (*S. aureus*) and (*E. coli*) using the agar disk diffusion method, and the corresponding inhibition zone diameters are summarized in Table 5 (Figures. 12 and 13) [28]. The results indicate that all synthesized complexes under the tested experimental conditions exhibited a moderate antibacterial activity against the two bacterial strains. Complex 3 is the most active of those tested and complex 1 has the least activity in this case. The overall activity trends are as follows: *S. aureus*: $3 > 4 > 5 > 2 \approx 1$, and *E. coli*: $3 > 4 > 2 > 5 > 1$.

The relatively high activity of complex 3 could be explained by the inclusion of dppe which increases lipophilicity, enabling interaction with bacterial cell membrane. In contrast, less active complex 1 may have the lower penetration and also weak interactions against to biological targets. These should all be considered preliminary assessments of antibacterial activity, based entirely on the agar disk diffusion assay. Due to the nature of these experiments, they

were not biological replicates, nor were statistics or minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) measured. Consequently, the available data should be viewed qualitatively rather than quantitatively. Regarding the resistance of bacteria, isolated bacteria are MDR (Multidrug resistant) It means that at least 3 groups of antibiotics have been detected as zero. Vancomycin and Meropenem showed no detectable inhibition under the experimental conditions. Such results may be attributed primarily to methodological factors including diffusion limitations, assay conditions, or experimental design parameters rather than failure of the extract to possess antibacterial activity at all. The lack of inhibition for the KBr control demonstrates that the activity detected is from the complexes and not from the supporting matrix. These results suggest there is a structure–activity relationship present within these complexes, with differences in ligand environment impacting their antibacterial activity.

Table 5: The diameter of inhibition complexes on *S. aureus* and *E. Coli* bacteria incubated for 24 hrs. at 37 °C

Compounds	Inhibition diameter zone (mm)	
	<i>S. aureus</i>	<i>E. Coli</i>
KBr	0	0
1	20	15
2	20	22
3	30	25
4	27	23
5	23	16
Vancomycin	...	...
Meropenem	...	...

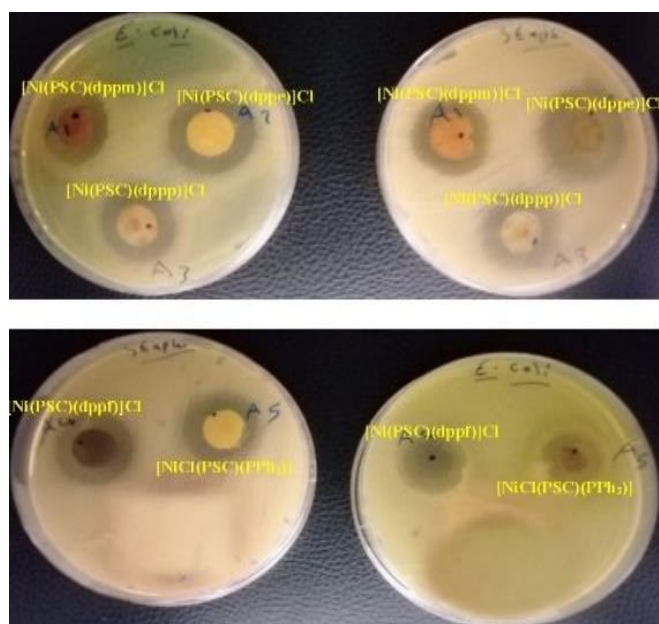


Figure 12: Antibacterial activity of synthesized Ni(II) complexes (1–4) against *S. aureus* and *E. coli* using the agar diffusion assay

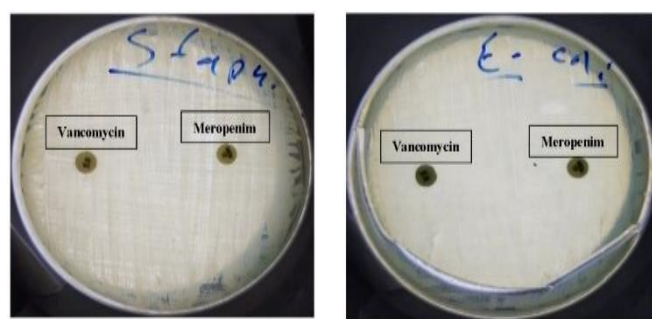


Figure 13: Antibacterial activity of the reference antibiotics Vancomycin and Meropenem against *S. aureus* and *E. coli* using the agar diffusion assay

4. Theoretical Study

4.1. DFT Studies

To gain more information about the electronic structure and reactivity of free ligands as well as their static Ni(II) complexes, DFT calculations were performed using Gaussian 09. Using the B3LYP functional, the ground-state geometries of the PSCH, the phosphine ligands, and their corresponding Ni(II) complexes were fully optimized without symmetry constraints. Non-metal atoms (free PSCH and tertiary phosphine ligands) were set at 6-31G(d) basis sets and the LANL2DZ effective core potential was applied to the nickel center in order to incorporate relativistic effects (Figures 14 and 15) [29,30].

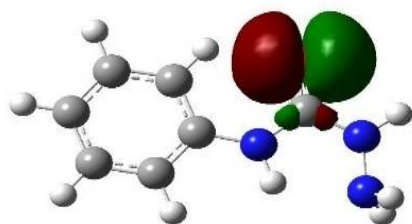
Frontier molecular orbital (FMO) analysis was done by computing the energies of Highest occupied molecular orbital (HOMO) and Lowest unoccupied molecular orbital (LUMO). The free ligands and their nickel complexes were analyzed for the computation of the HOMO–LUMO energy gap ($\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$). The value of this energy gap reflects the stability and reactivity of the studied species; a larger gap is indicative of higher stability and lower reactivity whereas a smaller gap depicts increased chemical activity. [31–33]. HOMO and LUMO energies were converted

into global reactivity descriptors, such as chemical hardness (η), chemical potential (μ) and chemical softness (S) via standard relationships. Chemical hardness was calculated according to equation: $\eta = (E_{\text{LUMO}} - E_{\text{HOMO}})/2$, a more quantitative measure of molecular stability. For complexes **1–4** (Figure 15), the HOMO energies (E_{HOMO}) are -3.5162, -3.9812, -8.5551, and -9.4258 eV, while the corresponding LUMO energies (E_{LUMO}) are -2.3923, -2.3439, -6.8381, and -2.0925 eV, respectively. The HOMO–LUMO energy gaps (ΔE) obtained are 1.1239, 1.6373, 1.717 and 7.3333 eV, respectively. The calculated electronic structure indicates that complex **4** has the largest energy gap of HOMO–LUMO and thus is the most stable, while complex **1** has the smallest one essentially indicating that it is relatively more reactive in nature among the investigated complexes. Among these values, two important quantum chemical parameters are global hardness and global softness that directly relate to the energy gap (where “hard” species correspond to larger gaps and “soft” counterparts have smaller gaps). Accordingly, complex **4** is predicted to be less reactive and predicted to be more stable, with higher hardness ($\eta = 3.6666$ eV), while complex **1** is more reactive and less stable, with lower hardness ($\eta = 0.5619$ eV). The data further suggest that complex **2** exhibits the highest dipole moment, whereas complex **3** demonstrates the lowest (Table 6) [34–36].

Table 6: Quantum chemical descriptors for the ligands and complexes (1–4)

Parameter	PSCH	PPh ₃	dppm	dppe	dppp	1	2	3	4
E_{HOMO} (eV)	-5.8666	-6.5341	-4.5151	-1.0574	-5.9883	-3.5162	-3.9812	-8.5551	-9.4258
E_{LUMO} (eV)	-0.0565	0.4157	1.9015	1.9989	0.2751	-2.3923	-2.3439	-6.8381	-2.0925
ΔE (eV)	5.8101	6.9498	6.4166	3.0563	6.2634	1.1239	1.6373	1.717	7.3333
μ (D)	5.5972	1.8185	2.3766	2.0473	3.3833	2.3879	4.2993	1.4075	3.6569
IP (eV)	5.8666	6.5341	4.5151	1.0574	5.9883	3.5162	3.9812	8.5551	9.4258
EA (eV)	0.0565	-0.4157	-1.9015	-1.9989	-0.2751	2.3923	2.3439	6.8381	2.0925
μ (eV)	-2.9615	-3.0592	-1.3068	0.4707	-2.8566	-2.9542	-3.1625	-7.6966	-5.7591
η (eV)	2.9050	3.4749	3.2083	1.5281	3.1317	0.5619	0.8186	0.8585	3.6666
S (eV)	0.1721	0.1438	0.1558	0.3272	0.1596	0.8898	0.6107	0.5824	0.1363

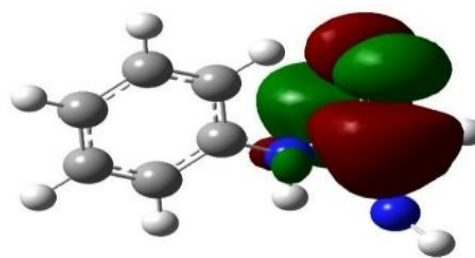
μ (D): Dipole moment (debye), IP: Ionization potential, EA: Electron affinity, μ : Electronic chemical potential, η : Chemical hardness, S : Chemical softness.



$E_{\text{HOMO}} = -5.8666$ eV

PSCH

$\Delta E = 5.8101$ eV



$E_{\text{LUMO}} = -0.0565$ eV

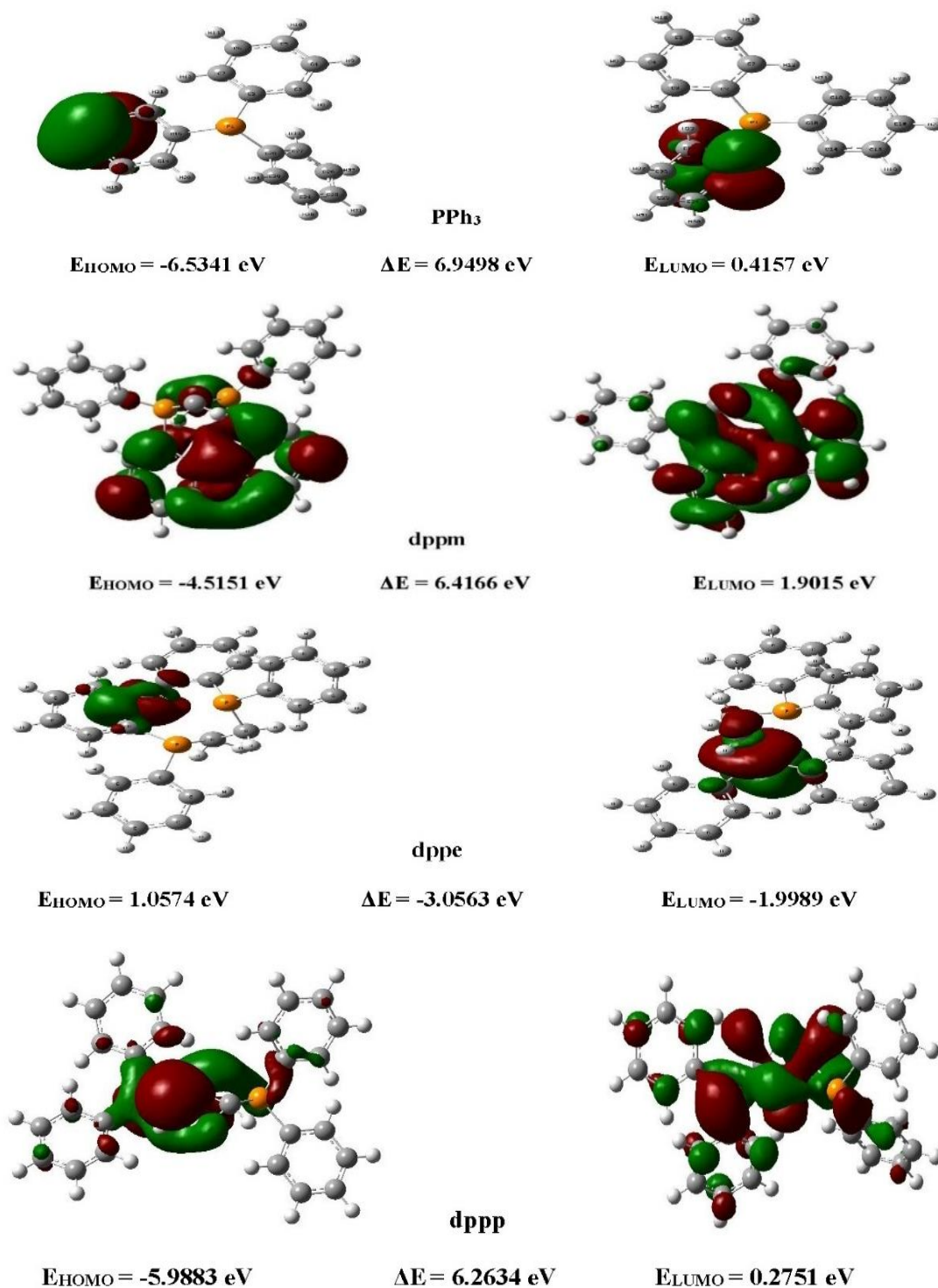


Figure 14: HOMO and LUMO contour plots and isosurface maps of the investigated ligands (PSC⁻, PPh₃, dppm, dppe, and dppp) calculated at an isosurface value of 0.02 a.u. The figure illustrates the electron density distribution of the frontier molecular orbitals, where HOMO represents electron-donating regions and LUMO represents electron-accepting regions

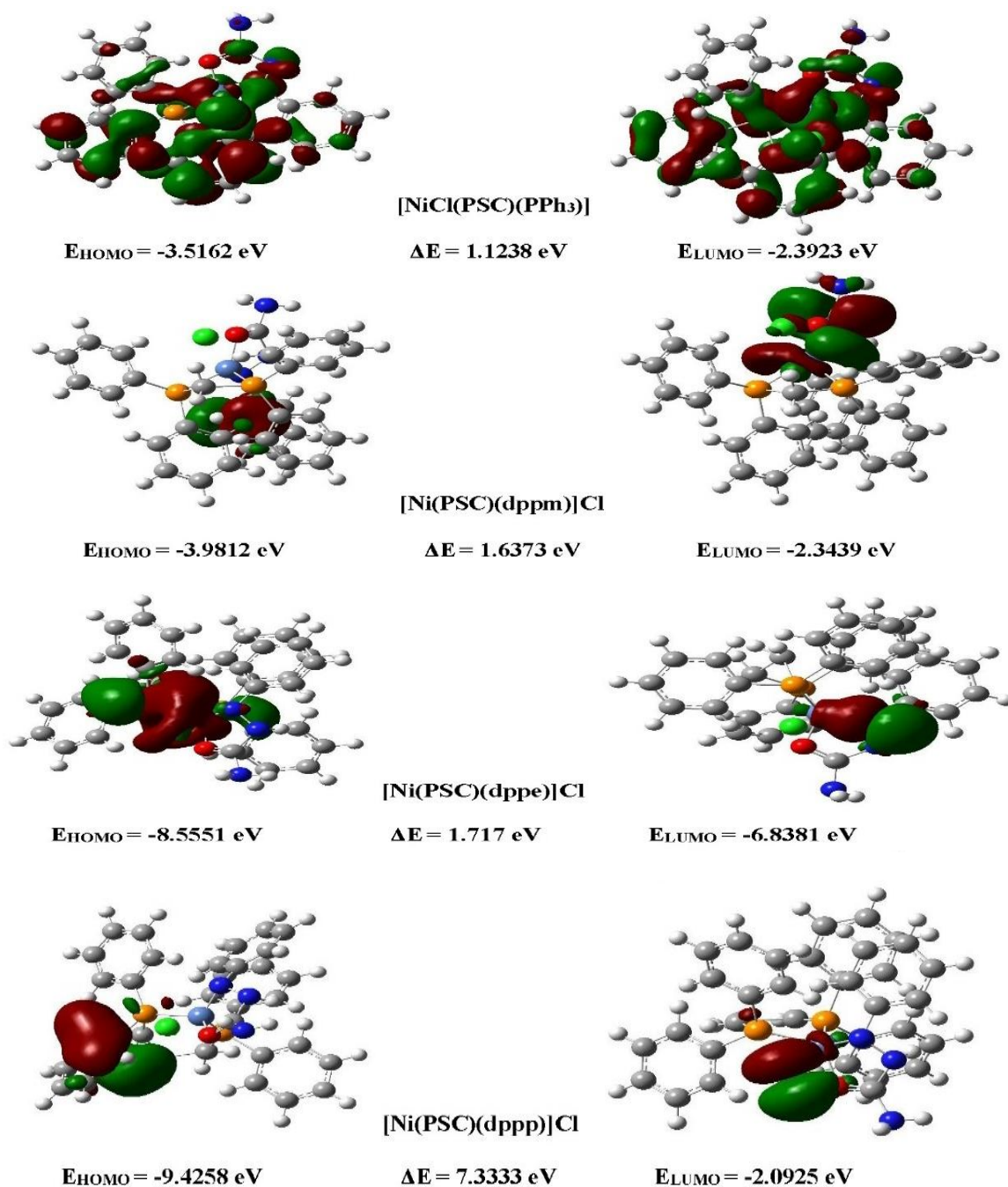


Figure 15: (HOMO) and (LUMO) contour plots and isosurface maps of Ni(II) complexes (1–4) calculated at an isosurface value of 0.02 a.u. The figure illustrates the frontier molecular orbital electron density distribution, where HOMO represents electron-donating regions and LUMO represents electron-accepting regions within each complex

4.2. NBO Analysis

NBO analysis was carried out to examine charge transfer interactions and donor–acceptor relationships between the ligands and the Ni(II) center. This gives quantitative data concerning the redistribution of electron density after complex formation. Natural atomic charges computed for the free PSCH and tertiary phosphine ligands and their corresponding Ni(II) complexes (1–4), are presented in Table 7 and Figure 16 [37].

It is observed in the series of complexes 1–4 was calculated NBO charges on the Ni metal display significant variation between +0.464 a.u. in complex 1 and negative values

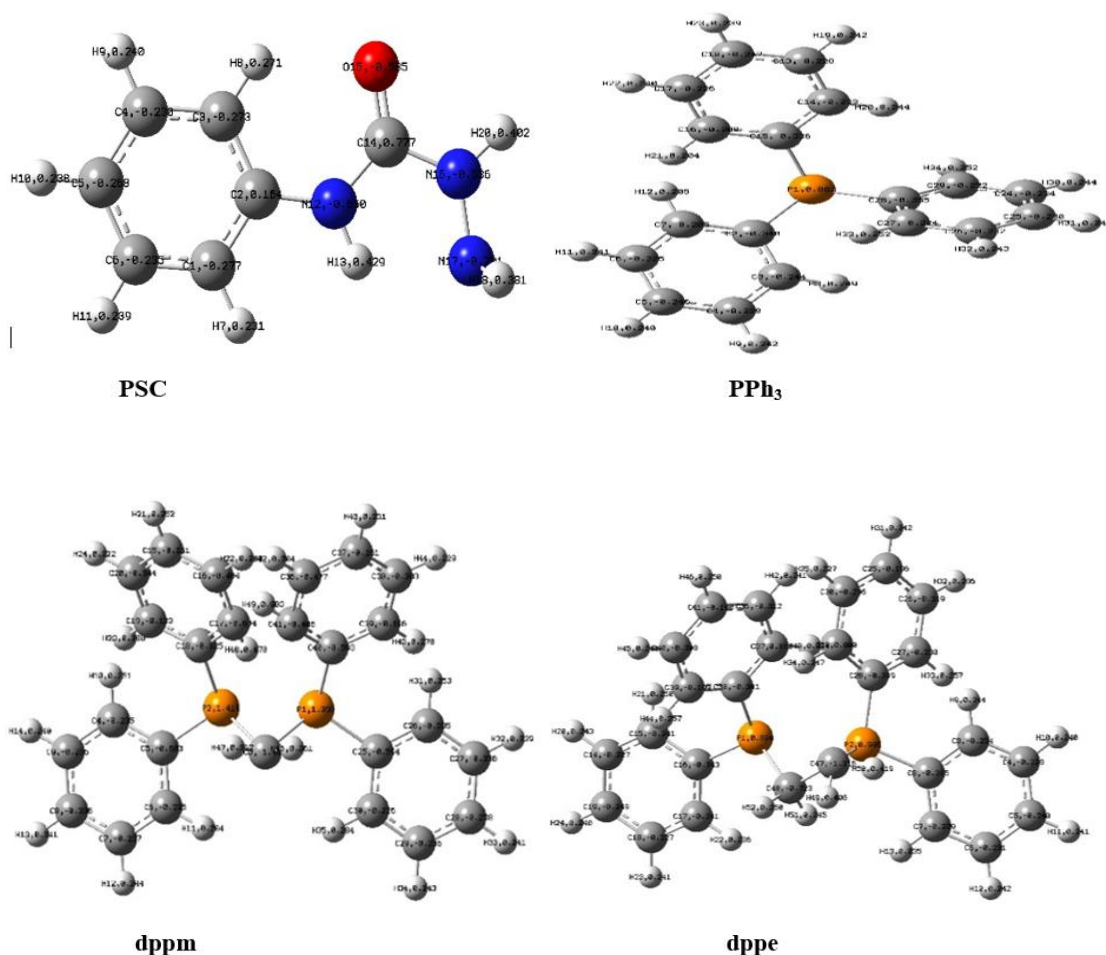
in complexes 2–4 (−0.506, −0.340, and −0.288 a.u., respectively). While all complexes formally contain nickel in the +2 oxidation state, NBO charges reflect the distribution of electron density rather than formal oxidation states and should be treated as such. The larger negative NBO charges we see for complexes 2–4 indicate that large amounts of electron density are piling up on the nickel center, as expected due to strong ligand-to-metal donation and significant metal–ligand covalent character. The difference between complex 1 and complexes 2–4 implies that the phosphine coordination environment has a strong impact on charge redistribution. Complex 1 also retains a net positive

nickel charge, which suggests more polarized electrons and therefore electron density at the metal center is lower. In contrast, the observed negative nickel charges for complexes **2–4** indicate better delocalization of electrons from PSC[−] and diphosphine ligands to Ni due to a more covalent nature in the Ni–N and Ni–P bonds. The stronger donor ability of chelating diphosphine ligands vs monodentate phosphine coordination is consistent with this trend, which emphasizes the important influence of ligand electronics on tuning electron density at the metal center. The nitrogen atoms in the PSC[−] ligand have decreased negative atomic charge (−0.307 to −0.549 a.u.) associated with complex formation from those of their respective free ligands (−0.536 and −0.650 a.u.), suggesting some donation of electron density toward metal center during the complex formation process [46]. In line with that, a decrease in the negative charge on the carbonyl oxygen in complexes **1, 2** and **4** supports its coordination involvement, while an increase of electron

density on oxygen which we observed in complex **3** suggests some additional intra-ligand charge redistribution because of varying metal–ligand orbital interactions. The phosphorus atomic charges of the phosphine ligands change further supporting electronic communication with the Ni(II) center. The increase in positive charge of the metal with respect to the free phosphines (PPh₃ and dppe) in complexes **1** and **3** indicates a net donation of electrons from phosphorus atoms into the metal center. On the contrary, in complexes **2** and **4** the decrease of the phosphorus atomic charge due to free phosphorus dpmm and dppp ligands demonstrates a better redistribution of density from the metal site towards ligand sized atoms [31,38]. In summary, NBO illustration demonstrates that variations in the atomic charge of Ni correlate with differences in ligand donor strength, degree of ligand-to-metal charge transfer and covalence character in metal–ligand bonding interactions.

Table 7: The NBO charge of ligands and complexes (1-4)

Atoms	PSCH	PPh ₃	dpmm	dppe	dppp	1	2	3	4
Ni	...	...	...	...	...	0.464	−0.506	−0.340	−0.288
O15	−0.585	...	...	...	...	−0.445	−0.559	−0.609	−0.354
N12	−0.650	...	...	...	...	−0.549	−0.497	−0.546	−0.407
N16	−0.536	...	...	...	...	−0.462	−0.502	−0.523	−0.307
N17	−0.701	...	...	...	...	−0.676	−0.918	−0.900	−0.583
P1	...	0.881	1.399	0.894	1.374	1.069	1.063	1.149	0.619
P2	...	...	1.419	0.996	1.426	...	1.048	1.143	1.024



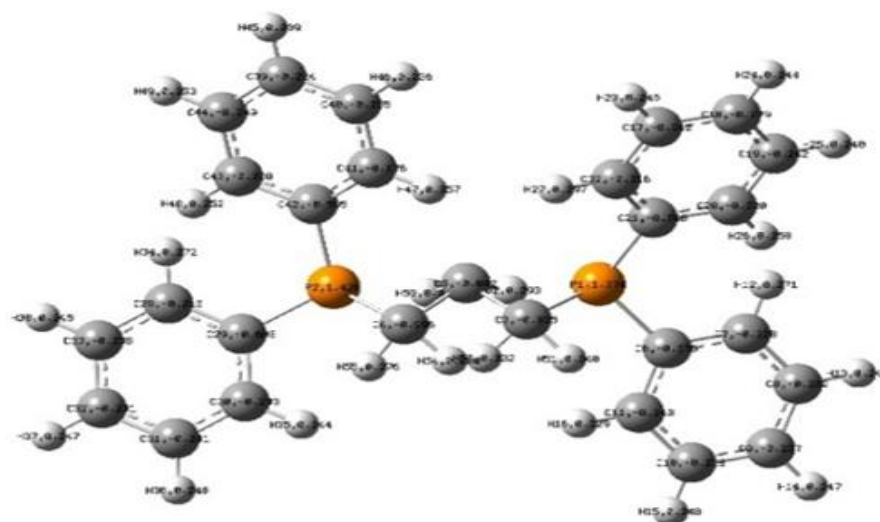
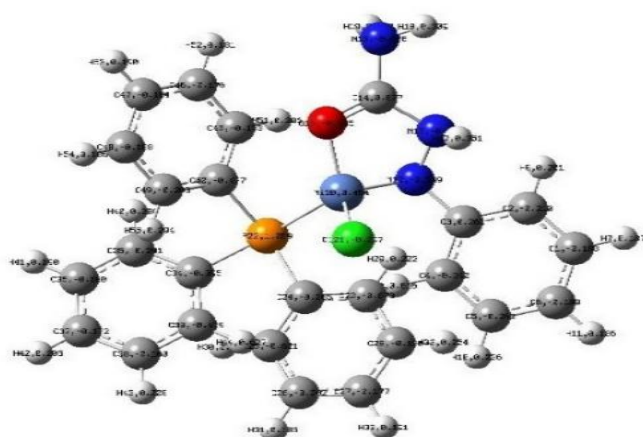
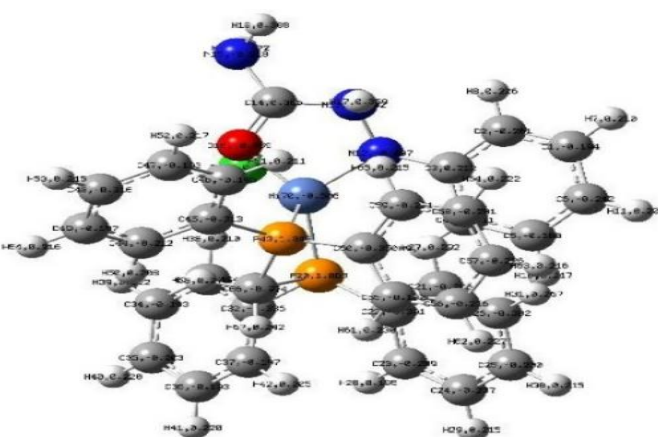
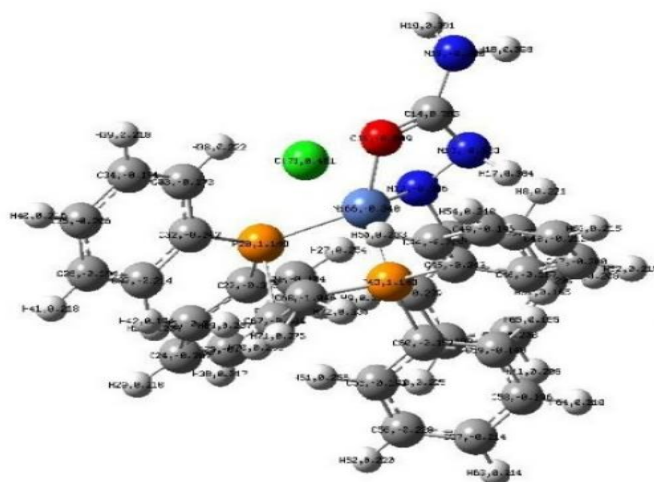
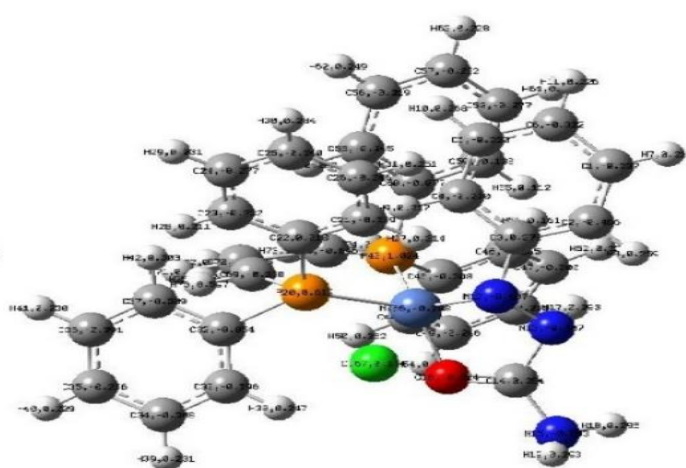
**dppp****[NiCl(PSC)(PPh₃)]****[Ni(PSC)(dppm)]Cl****[Ni(PSC)(dppe)]Cl****[Ni(PSC)(dppp)]Cl**

Figure 16: NBO atomic charges of the free ligands and Ni(II) complexes (1–4), illustrating the redistribution of electron density upon coordination. The data highlight changes in atomic charges at donor atoms (N, O, and P) and the Ni center, reflecting ligand-to-metal charge transfer and variations in metal–ligand bonding interactions

4.3. Molecular Electrostatic Potential Analysis (MEP)

MEP maps provide useful information about the charge distribution, molecular geometry and reactive site of chemical system. These maps allow to identify regions that are susceptible to nucleophilic and electrophilic attacks. Applied visualizations of electrostatic potential mirrors this behavior, with red regions corresponding to negative electrostatic potentials (electron-rich) and blue regions corresponding to positive electrostatic potentials (electron-deficient) in the molecule (MEPs) [39]. Calculations of MEP surfaces of free ligands and their respective Ni(II) complexes were performed using Gaussian 09 software, as illustrated in (Figure 17) [35]. For the uncoordinated ligands, negative electrostatic potential (red) regions are localized chiefly on the carbonyl oxygen atom of PSCH and the phosphorus atoms of phosphine, along with showing first signs for electron-rich sites. On the other hand, areas with positive

electrostatic potential (blue) are largely located around hydrogen and nitrogen atoms which represents electron-deficient regions. An analysis of the MEP maps of complexes 1–4 reveals a clear redistribution of electron density upon their coordination. Finally, the carbonyl oxygen atom of PSC- still demonstrates a localization of high negative electrostatic potential so we can confirm it as an electron-donating site essential for charge separation [34]. On the other hand, the two nitrogen atoms show less positive potential regions around them and these indicate that they play a different role in coordination with a metal center. Higher electron density localized on the oxygen compared to nitrogen is consistent with its higher electronegativity. Regions with negative electrostatic potential favor electrophilic attack, while the positive regions are nucleophilic forces. Thus the MEP calculation supports the suggested coordination mode and points to carbonyl oxygen atom as a preferred electrophilic center in these complexes [39].

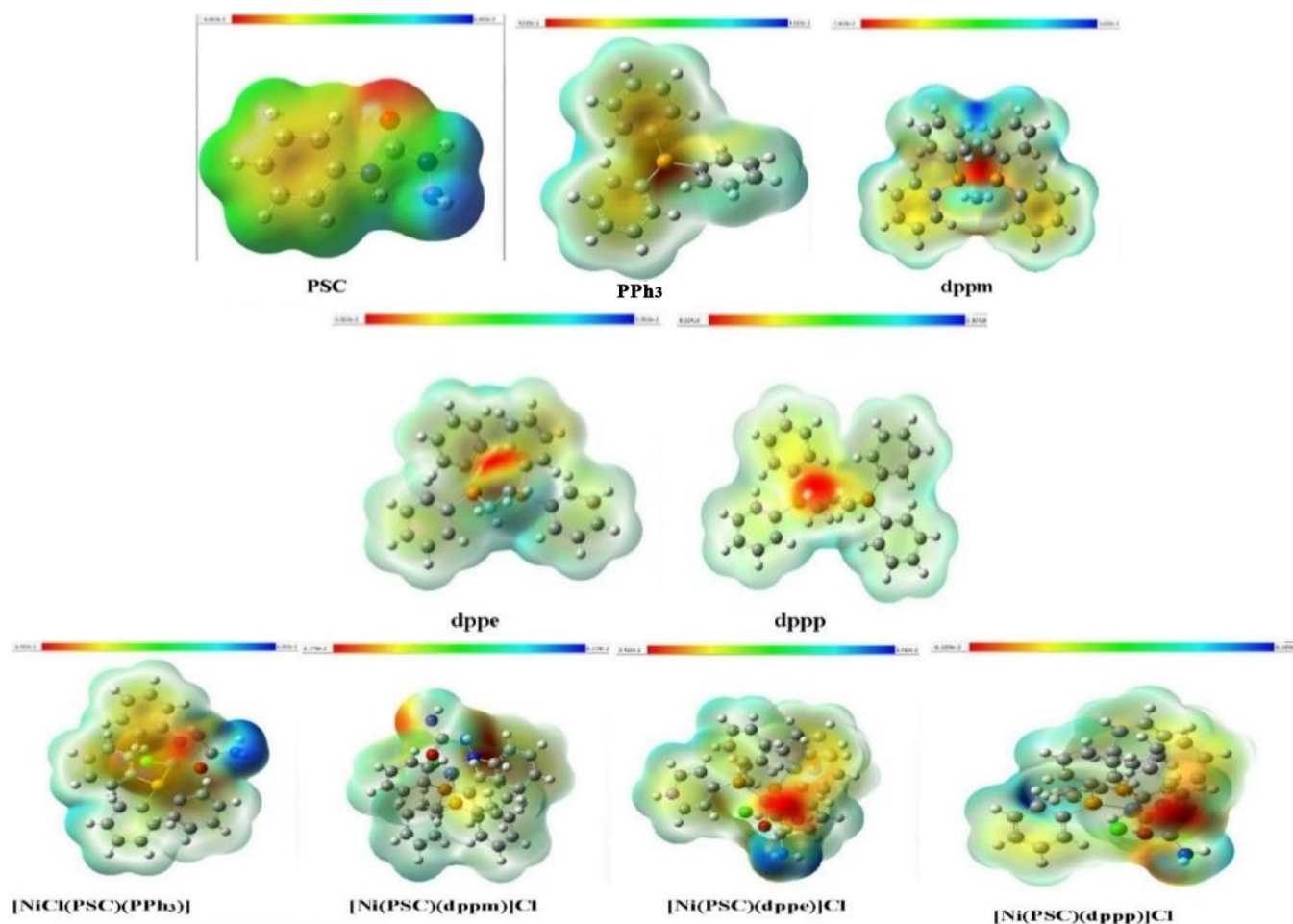


Figure 17: MEP surfaces of the optimized structures of the free ligands and Ni(II) complexes (1–4), mapped in atomic units (a.u.). The MEP surfaces illustrate the charge distribution within each molecule, where red regions indicate electron-rich (negative potential) sites, blue regions indicate electron-poor (positive potential) sites, and intermediate colors represent neutral regions. These maps were generated from the optimized geometries to visualize reactive sites for electrophilic and nucleophilic attack

5. Conclusions

This work describes the synthesis and characterization of a new series of mixed-ligand Ni(II) complexes with PSCH as well as some tertiary phosphine ligands. This work to the best of our knowledge reports the first PSC⁻ mediated by tertiary phosphines within a Ni(II) complex. Spectroscopic, analytical, and magnetic measurements suggest that the products are proposed to a distorted square-planar, four-coordinate Ni(II) complexes in which PSC⁻ acts as a bidentate chelating ligand coordinating to nickel metal through both its nitrogen and carbonyl oxygen donor atoms while phosphine ligands coordinate through phosphorus atoms.

The reactivity of the other complexes can be compared through complementary DFT, NBO and MEP studies confirming that complex 4 is indeed more stable and less reactive than the other two analogues. The preliminary antibacterial screening indicated that these complexes have different bacteriostatic action on *S. aureus* and *E. coli*, complex 3 being the most active among all three in relation to the applied experimental conditions.

This work extends the range of coordination chemistry accessible to semicarbazide-based ligands and lays groundwork for future research in this area. Future studies using single-crystal X-ray diffraction and further biological evaluations are needed to verify potential structures and evaluate their biological properties.

Acknowledgments

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Data availability The datasets created and analyzed for this investigation are available upon reasonable request from the corresponding author.

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