Asian Journal of Chemistry; Vol. 33, No. 8 (2021), 1749-1756

ASIAN JOURNAL OF CHEMISTRY

https://doi.org/10.14233/ajchem.2021.23214

Spectral, Theoretical and Biological Studies of 3-((4-Mercaptophenyl)imino)-1-phenylindolin-2-one Schiff Base and Its Organotellurium(IV) Complexes

MANISH KUMAR[1], POONAM JANGRA DAROLIA[1], NIDHI ANTIL[1], MAHAK DALAL[1], JITENDER NARWAL[2], K.K. VERMA[1] and SAPANA GARG[1,*]

[1]Department of Chemistry, Maharishi Dayanand University, Rohtak-124001, India
[2]Department of Chemistry, Janta Vidya Mandir Ganpat Rai Rasiwasia College, Charkhi Dadri-127306, India

*Corresponding author: E-mail: sapanagarg1511@gmail.com

Received: 23 March 2021; *Accepted*: 30 April 2021; *Published online*: 26 July 2021; AJC-20423

Schiff base ligand (3-((4-mercaptophenyl)imino)-1-phenylindolin-2-one) of 1-phenylindoline-2,3-dione and 4-aminothiophenol was synthesized by refluxing. Organotellurium(IV) complexes of type ($RTeCl_3$.NPhIATP and R_2TeCl_2.NPhIATP, where R = 4-hydroxyphenyl, 4-methoxyphenyl and 3-methyl-4-hydroxyphenyl, NPhIATP = Schiff base ligand). The ligand and its organotellurium(IV) complexes (**9a-f**) were characterized by FT-IR, molar conductance, elemental analyses, UV-vis, mass, ^1H & ^{13}C NMR spectral studies. Geometry of all the compounds were optimized and octahedral geometry have been proposed for all the tellurium(IV) complexes. Molecular docking was studied to find the binding interactions between ligand (NPhIATP) and receptor proteins: *E. coli* (3t88) and *S. aureus* (3ty7). The antimicrobial activity of ligand and its tellurium(IV) complexes have been screened against bacteria and fungi. All the organotellurium(IV) complexes complexes showed good activity to ligand towards different studied microorganisms.

Keywords: 1-Phenylindoline-2,3-dione, Organotellurium(IV) complexes, *p*-Aminothiophenol, Antimicrobial activity.

INTRODUCTION

Interest in the field of bioinorganic chemistry of Schiff base metal complexes [1,2] have been increased recently. They are biologically important classes as they show physiological activity [3] like anticancer [4,5], anti-inflammatory [6,7], antimicrobial [8-15] activities, *etc.* Isatin (indole-2,3-dione) and its derivatives have long been known as a cheap precursor for the drug synthesis. Isatin based Schiff bases [16-20] show a variety of biological and pharmacological activities. The presence of additional donor sites makes it more flexible and versatile towards metal ions. It is well acknowledged that organotellurium(IV) complexes [21-23] possess remarkable biological activities. Steric and electronic organic groups on tellurium impart substantial influence on their structural characteristics.

Based on the above facts, in this work, a new series of organotellurium(IV) complexes ($RTeCl_3$/R_2TeCl_2.NPhIATP) of Schiff base obtained from condensation reaction of 1-phenylindoline-2,3-dione and 4-aminothiophenol were synthesized, characterized by various spectroscopic techniques and examined for their antimicrobial activity against reported bacterial and fungal strains.

EXPERIMENTAL

1-Phenylindole-2,3-dione, phenol, tellurium tetrachloride, 4-aminothiophenol, anisole, 2-methylphenol were of analytical grade and purchased from Sigma-Aldrich, USA. The solvents were further purified by standard procedures [24,25]. All the reactions were carried out in dry atmosphere of N_2.

The elemental analyses for C, H and N were determined by using CHNS analyzer at Central Instrumentation Laboratory, M.D. University. The molar conductance of complexes was calculated by conductivity cell (cell constant = 1.017) on bridge type conductivity MICROSIL. FT-IR of the Schiff base ligand and its complexes were measured on Thermoscientific Nicolet iS50 spectrophotometer using KBr pallets and polyethylene pallets. UV-Visible spectra were obtained with Shimadzu UV-3600 Plus using $BaCl_2$ pallets. The EI-MS mass spectra of the compounds were recorded on mass analyzer. ^1H & ^{13}C NMR

were recorded on a 400 NMR Spectrometer (Bruker Avance II) in DMSO-d_6 and $Si(CH_3)_4$ was taken as reference. Tellurium chloride was estimation by Volhard's method.

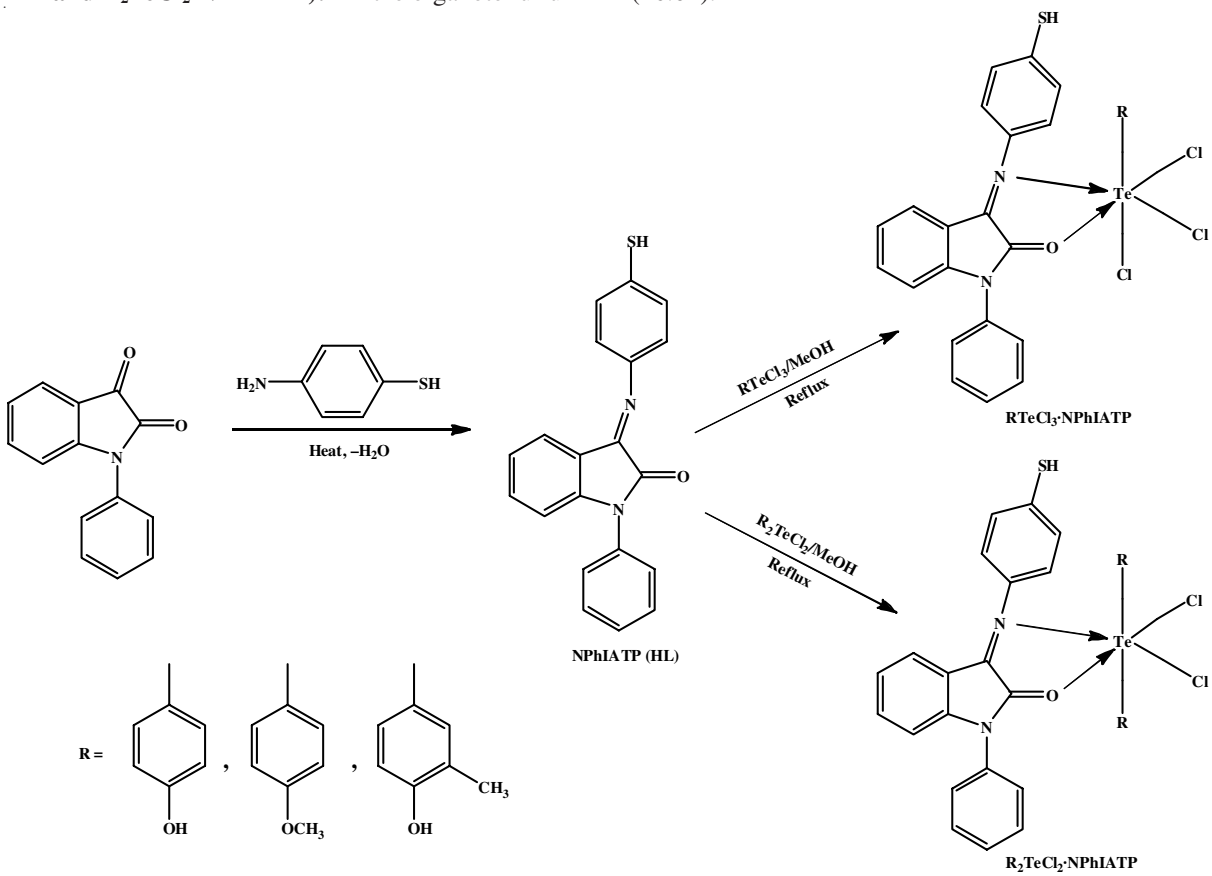
Synthesis of (3-((4-mercaptophenyl)imino)-1-phenylindolin-2-one) Schiff base ligand (NPhIATP or HL): Schiff base (NPhIATP) was synthesized by the condensation reaction of 1-phenylindoline-2,3-dione (15mmol) and *p*-aminothiophenol (15mmol) in absolute ethanol (50 mL), the reaction mixture was refluxed on water bath for 3 h with continuous stirring. On cooling, orange red coloured precipitates separate out. The orange red coloured precipitates formed were filtered, recrystallized with ethanol and dried in vacuum desiccator over anhydrous $CaCl_2$ [18,21]. Colour: orange red, yield: 74.29% (3.88 g), *m.w.*: 330.42 g/mol; m.p.: 154-156 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 6.78-7.67 (m, 13H, Ar-H), 3.44 (s, 1H, S-H). ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 162.72 (C=O), 157.93 (C=N), 111.22-151.72 (Ar-C). IR (KBr, ν_{max}, cm^{-1}): 3092 (Ar-CH), 2581 (S-H), 1745 (C=O), 1632 (C=N), 1178 (C-S). MS (EI, 70 eV) *m/z* (%): 331.10 (100). Elemental analysis of NPhIATP ($C_{20}H_{14}N_2OS$) calcd. (found) %: C, 72.70 (73.02); H, 4.27 (4.11); N, 8.48 (8.25).

Synthesis of organotellurium(IV) trichlorides ($RTeCl_3$) and diorganotellurium(IV) dichlorides (R_2TeCl_2): All the organotellurium(IV) chlorides ($RTeCl_3$ and R_2TeCl_2; where R = 4-hydroxyphenyl, 4-methoxyphenyl and 3-methyl-4-hydroxyphenyl) were synthesized by reaction of $TeCl_4$ with *o*-cresol, anisole and phenol, respectively as reported in literature [26-30].

Synthesis of organotellurium(IV) complexes ($RTeCl_3$·NPhIATP and R_2TeCl_2·NPhIATP): All the organotellurium (IV) complexes had been synthesized by refluxing of equimolar ratio of hot methanolic solutions of $RTeCl_3$/R_2TeCl_2 with Schiff base ligand (NPhIATP) for 4 h on hot plate with magnetic stirrer. Reduced the extra volume of methanol in vacuum kept the resulting solution for precipitation at room temperature. After 6-7 days, coloured precipitates were obtained, filtered, washed with petroleum ether and dried in vacuum desiccator over anhydrous $CaCl_2$ (**Scheme-I**).

$RTeCl_3$·NPhIATP (4-hydroxyphenyl) (9a): Colour: brown, Yield: 87.04% (1.00 g); *m.w.* 657.96 g/mol; m.p.:124-127 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 10.16 (s, 1H, Ar-OH), 6.93-8.25 (m, 17H, Ar-H) 3.44 (s, 1H, S-H). ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 183.26 (C=O), 160.80 (C_2), 158.59 (C-OH), 111.22-151.84 (Ar-C). IR (KBr, ν_{max}, cm^{-1}): 3365 (O-H), 3061 (Ar-CH), 2580 (S-H), 1732 (C=O), 1608 (C=N), 1176 (C-S), 495 (Te-O), 287 (Te-N). Elemental analysis of **9a** ($C_{26}H_{19}N_2O_2SCl_3Te$) calcd. (found) %: C, 47.50 (47.24); H, 2.91 (3.10); N, 4.26 (4.24); Te, 19.41 (19.13), Cl, 16.18 (16.39).

$RTeCl_3$·NPhIATP (4-methoxyphenyl) (9b): Colour: red brown, Yield: 82.14% (1.10 g); *m.w.*: 671.49 g/mol; m.p.: 119-121 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 6.82-8.24 (m, 17H, Ar-H), 3.81 (s, 3H, OCH_3), 3.44 (s, 1H, S-H). ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 183.25 (C=O), 160.19 (C=N), 111.22-151.85 (Ar-C), 55.95 (OCH_3). IR (KBr, ν_{max}, cm^{-1}): 3059 (Ar-CH), 2927 (C-H), 2572 (S-H), 1738 (C=O), 1607 (C=N), 1179 (C-S), 490 (Te-O), 291 (Te-N). Elemental analysis for **9b** ($C_{27}H_{21}Cl_3N_2O_2STe$) calcd. (found) %: C, 48.29 (48.45); H, 3.15 (3.32); N, 4.17 (4.02); Te, 19.00 (18.75); Cl, 15.84 (16.04).



Scheme-I: Synthetic route of organotellurium(IV) complexes

$RTeCl_3$·NPhIATP (3-methyl-4-hydroxyphenyl) (9c): Colour: yellow; yield: 72.75 % (0.97g). *m.w.*: 671.49 g/mol; m.p.: 131-133 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 10.12 (s, 1H, Ar-OH), 6.83-8.23 (m, 17H, Ar-H), 2.14 (s, 3H, -CH_3); ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 183.20 (C=O), 160.74 (C=N), 158.41 (C-OH), 111.22-159.32 (Ar-C), 16.56 (CH_3). IR (KBr, ν_{max}, cm^{-1}): 3349 (O-H), 3061 (Ar-CH), 2923 (C-H), 2581 (S-H), 1717 (C=O), 1606 (C=N), 1179 (C-S), 492 (Te-O), 290 (Te-N). Elemental analysis of **9c** ($C_{27}H_{21}Cl_3N_2O_2STe$) calcd. (found) %: C, 48.29 (48.24); H, 3.15 (2.99); N, 4.17 (3.98); Te, 19.00 (18.83); Cl, 15.84 (15.69).

R_2TeCl_2·NPhIATP (4-Hydroxyphenyl) (9d): Colour: brown, yield: 86.54% (1.24 g), *m.w.*: 715.12 g/mol; m.p.: 129-131 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 10.14 (s, 2H, Ar-OH), 6.91-8.25 (m, 21H, Ar-H), 3.44 (s, 1H, S-H). ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 183.26 (C=O), 160.79 (C=N), 158.52 (C-OH), 111.23-151.84 (Ar-C). IR (KBr, ν_{max}, cm^{-1}) = 3358 (O-H), 3058 (Ar-CH), 2578 (S-H), 1736 (C=O), 1608 (C=N), 1177 (C-S), 495 (Te-O), 288 (Te-N). Elemental analysis for **9d** ($C_{32}H_{24}Cl_2N_2O_3STe$) calcd. (found) %: C, 53.75 (54.01); H, 3.38 (3.26); N, 3.92 (3.99); Te, 17.84 (18.12); Cl 9.92 (10.13).

R_2TeCl_2·NPhIATP (4-methoxyphenyl) (9e): Colour: dark brown, yield: 85.17% (1.27g), *m.w*.: 743.17 g/mol, m.p.: 103-106 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 6.83-8.24 (m, 21H, Ar-H), 3.83 (s, 6H, OCH_3), 3.44 (s, 1H, S-H). ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 183.24 (C=O), 160.20 (C=N), 111.22-158.50 (Ar-C), 55.95 (s, 6H, OCH_3). IR (KBr, ν_{max}, cm^{-1}): 3058 (Ar-CH), 2926 (C-H), 2578 (S-H), 1738 (C=O), 1607 (C=N), 1179 (C-S), 492 (Te-O), 290 (Te-N). Elemental analysis for **9e** ($C_{34}H_{28}Cl_2N_2O_3STe$) calcd. (found) %: C, 54.95 (55.14); H, 3.80 (4.06); N, 3.77 (3.89); Te, 17.17 (17.14); Cl, 9.54 (9.34).

R_2TeCl_2·NPhIATP (3-methyl-4-hydroxyphenyl) (9f): Colour: yellow, yield: 73.67% (1.09 g), *m.w.*: 743.17 g/mol, m.p.: 101-103 ºC. ^{1}H NMR (600 MHz, DMSO-d_6) δ ppm: 10.21 (s, 2H, Ar-OH), 6.92-8.24 (m, 19H, Ar-H), 2.14 (s, 6H, -CH_3). ^{13}C NMR (600 MHz, DMSO-d_6) δ ppm: 183.20 (C=O), 160.72 (C=N), 158.41 (C-OH), 111.22-151.85 (Ar-C), 16.56 (CH_3). IR (KBr, ν_{max}, cm^{-1}): 3350 (O-H), 3061 (Ar-CH), 2923 (C-H), 2581 (S-H), 1717 (C=O), 1606 (C=N), 1177 (C-S), 492 (Te-O), 291 (Te-N). Elemental analysis for **9f** ($C_{34}H_{28}Cl_2N_2O_3STe$) calcd. (found) %: C, 54.95 (54.87); H, 3.80 (3.87); N, 3.77 (3.73); Te, 17.17 (16.98); Cl, 9.54 (9.78).

Computational method: To rationalize the experimental results, a theoretical procedure was performed with Avogadro software. The gas phase geometries of ligand and complexes were optimized and distorted octahedral geometry were purposed for all the organotellurium(IV) complexes. HOMO-LUMO energy and other chemical quantum parameters were determined by using ORCA visualization program with Avogadro program.

Molecular docking studies: The three-dimensional structures of receptors of proteins: *E. coli* (3t88) and *S. aureus* (3ty7) were downloaded from RCSB PDB protein data bank website. Schiff base ligand (NMeIATP) were drawn in Avogadro 4.0 program and export for pdb files into Pymol software. The Autodock vina tools were used for docking of reported receptors and ligand. The docking analysis results were visualized with the help of Pymol software.

***in vitro* Antimicrobial activity:** Antibacterial activity of the ligand and its organometallic complexes were tested against the bacterial species of three Gram-positive bacteria such as *Bacillus cereus*, *Xanthomonas campestris* and *Staphylococcus aureus* and one Gram-negative bacteria *Escherichia coli* using agar well diffusion method. The ligands and complexes were also tested against the fungal species *Candida albicans*, *Fusarium oxysporum*, *Macrophomina phaseolina* and *Rhizoctonia solani*. Fungal cultures were grown on potato dextrose agar and bacterial cultures were grown on Mueller Hilton agar.

Cycloheximide and tetracycline were used as the standard antifungal and antibacterial agents, respectively. The compounds were prepared in DMSO. 18-24 h single colonies on agar plates were used to prepare the bacterial suspension with the turbidity of 1.5×10^8 CFU/mL were measured at 600 nm. Bacterial and fungal suspension (100 µL) were inoculated and spreaded on Mueller-Hinton agar plates and potato dextrose agar, respectively under aseptic conditions. Wells with diameter of 6 to 8 mm were punched aseptically with cork borer and wells were filled with 50 µL of all compounds and incubated for 24 h at 37 ºC for bacteria and 72 h for fungi. The diameter of growth inhibition zones was measured after the incubation period. All the experiments were performed in triplicate.

RESULTS AND DISCUSSION

The newly synthesized organotellurium(IV) complexes ($RTeCl_3$·NPhIATP and R_2TeCl_2·NPhIATP) were coloured amorphous solids, soluble in ethanol, methanol, DMSO and DMF. Schiff base (NPhIATP) and organotellurium(IV) complexes were analyzed for their physical properties and analytical data.

Conductance studies: Molar conductivity (Λ_M) of all organotellurium complexes (**9a-f**) at *ca.* 10^{-3} M at 25 ºC were measured in DMSO. The molar conductance (Λ_M) values lie in the range of 38.65-66.19 ohm^{-1} cm^2 mol^{-1}, which predicts them as weak electrolytes [31-33] probably due to the ionization into R_2TeCl_2.$NPhIATP^{+}$/R_2TeCl·$NPhIATP^{+}$ and Cl^- in DMSO.

IR spectra: The FT-IR spectrum of ligand exhibited a broad band at 2581 cm^{-1} attributed to S-H vibrations [34]. This band is also present in the spectra of the complexes suggesting that S-H group has no participation in complex formation. Two strong bands at 1745 and 1632 cm^{-1} are assigned to carbonyl [35] (C=O) and imine [36,37] (C=N) stretching frequencies in free ligand (Fig. 1a). On complexation, these bands shifted to lower frequency by 15-20 cm^{-1} indicating involvement of imine nitrogen and carbonyl oxygen of 1-phenylizatin ring to tellurium ion. This is further upheld by appearance of two new bands showing characteristic Te-N and Te-O bands [11,14] in the range of 495-490 cm^{-1} and 292-287 cm^{-1} (Fig. 1b). Thus, ligand (NPhIATP) acts as a bidentate NO donor.

Mass spectra: The mass spectrum of Schiff base ligand (NPhIATP) showed molecular ion peak at *m/z* = 331.09 indicating the presence of $[M-H]^+$ which is equivalent to molecular mass [38] of the ligand. The peaks at *m/z* 303.08, 224.06 and 145.99 are due to important fragments due to loss of thiol and phenyl rings, which describe the formation of Schiff base. The mass spectra of complexes **9a**, **9b**, **9c**, **9d**, **9e** and **9f** are 658.01, 672.09, 671.98, 716.08, 744.09 and 745.09, respectively holds

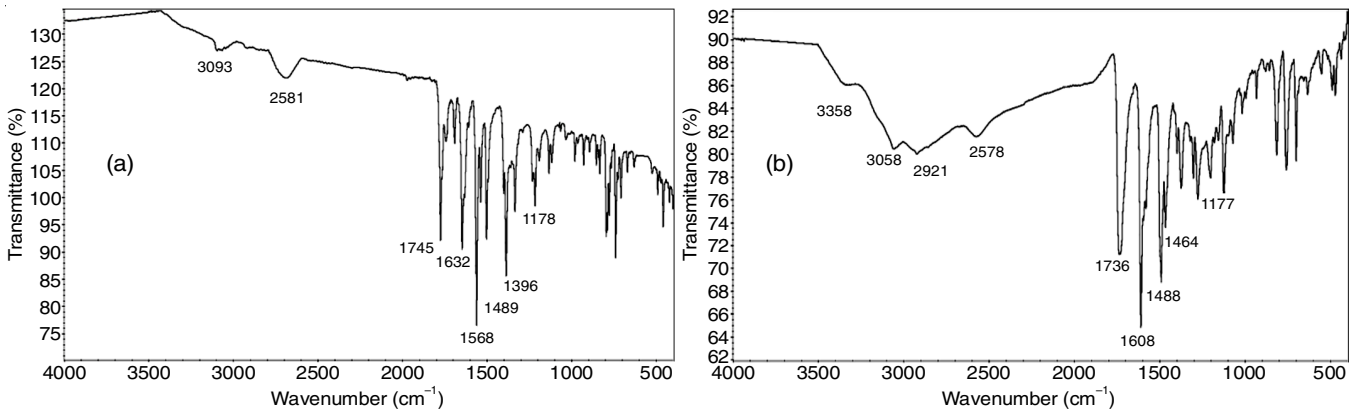


Fig. 1. FT-IR spectrum of the (a) ligand (NPhIATP) and (b) R_2TeCl_2·NPhIATP (**9d**)

good with the molecular mass of the organotellurium(IV) complexes predicts the 1:1 molar ratio of ligand and $RTeCl_3/R_2TeCl_2$.

UV-visible spectra: The significant UV-visible spectral bands [39-41] of ligand (NPhIATP) and organotellurium(IV) complexes are shown in Fig. 2. The UV-visible spectrum of Schiff base (NPhIATP) showed three bands at 223, 292 and 439 nm, which assigned to π-π^* transition of aryl rings, n-π^* transition of heteroatom groups and charge transfer transitions with in indole moiety, respectively. In the spectra of the organotellurium(IV) complexes, all the bands showed bathochromic shifts and absorbed in the range of 236-240 nm, 302-316 nm and 460-463 nm (Table-1). These shifts in the bands suggest the coordination to tellurium from ligand *via* imine nitrogen and carbonyl oxygen.

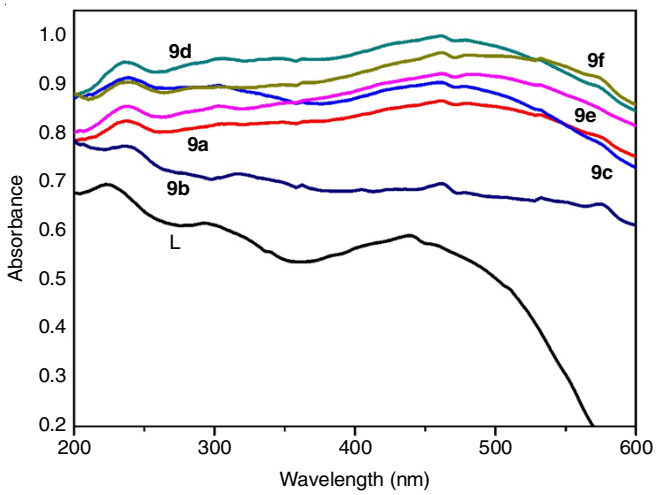


Fig. 2. UV-vis spectra of NPhIATP and organotellurium(IV) complexes

TABLE-1
UV-VISIBLE SPECTRA OF NPhIATP AND ITS ORGANOTELLURIUM(IV) COMPLEXES

Compound	λ_{max} (π-π^*) nm	λ_{max} (n-π^*) nm	λ_{max} (CT) nm
NPhIATP	223	292	439
9a	237	306	462
9b	239	303	461
9c	238	316	460
9d	236	304	461
9e	238	305	462
9f	240	302	463

^{1}H & ^{13}C NMR spectra: The ^{1}H NMR spectrum of ligand exhibited a singlet [34] appeared at δ 3.44 ppm and a multiplet in the range δ 6.78-7.67 ppm due to aromatic protons [42-44]. In the ^{1}H NMR spectra of the synthesized complexes (**9a**, **9c**, **9d** and **9f**), a singlet at δ 10.12-10.16 ppm was observed belonging to O-H proton of R group in $RTeCl_3/R_2TeCl_2$. In spectra, the aromatic protons show deshielding and observed at δ 6.81-8.29 ppm. Also, appearance of singlet at δ 3.44-3.46 ppm confirmed that S-H group does not participate in complexation (Fig. 3).

^{13}C NMR spectrum of ligand exhibited C=O and C=N signals at δ 162.72 and δ 157.93 ppm, respectively, which show downfield shift and observed at δ 183.26 and δ 160.19-160.80 ppm confirmed the coordination of imine nitrogen and carbonyl oxygen from ligand to tellurium metal [42]. Spectra of all compounds show a range of δ 111.22-151.85 ppm attributed to aromatic carbons, 16.56 ppm for -CH_3 and 55.95 ppm for -OCH_3 carbons.

DFT calculations: Optimized structures of NPhIATP and organotellurium(IV) complexes **9a**, **9d** by using Avogadro 4.0 software are shown in Fig. 4. In view of hexacoordination of complex **9a**, the tellurium metal is 2.062 Å and 2.015 Å away from imine nitrogen and carbonyl oxygen, respectively. The two Te-Cl bonds (2.413 Å) are *trans* to each other. One Te-Cl bond and one Te-C bond have bond length 2.412 Å and 2.182 Å, respectively to complete the coordination sphere around metal. The optimized structures of the complexes suggest distorted octahedral geometry resemble with spectroscopic characterization. In complex **9a**, the actual bond length and angels are approaching to their optimized values (Fig. 4). The C=N and C=O bond lengths are 1.294 Å and 1.221 Å, respectively in ligand and change in complexes as reported in Table-2. This enhancement in C=N and C=O bond lengths indicates the coordination of Schiff base ligand *via* N and O atoms.

Avogadro with ORCA visualization program with def2-SVP set is used to calculate the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) for ligand, complexes **9a** and **9d** and energy values are presented in Table-3. Lesser value of the energy gap [45] (ΔE) between HOMO and LUMO explains the greater reactivity of the complexes than ligand. HOMO is localized on the π-moieties of indole and aryl rings, while LUMO is localized

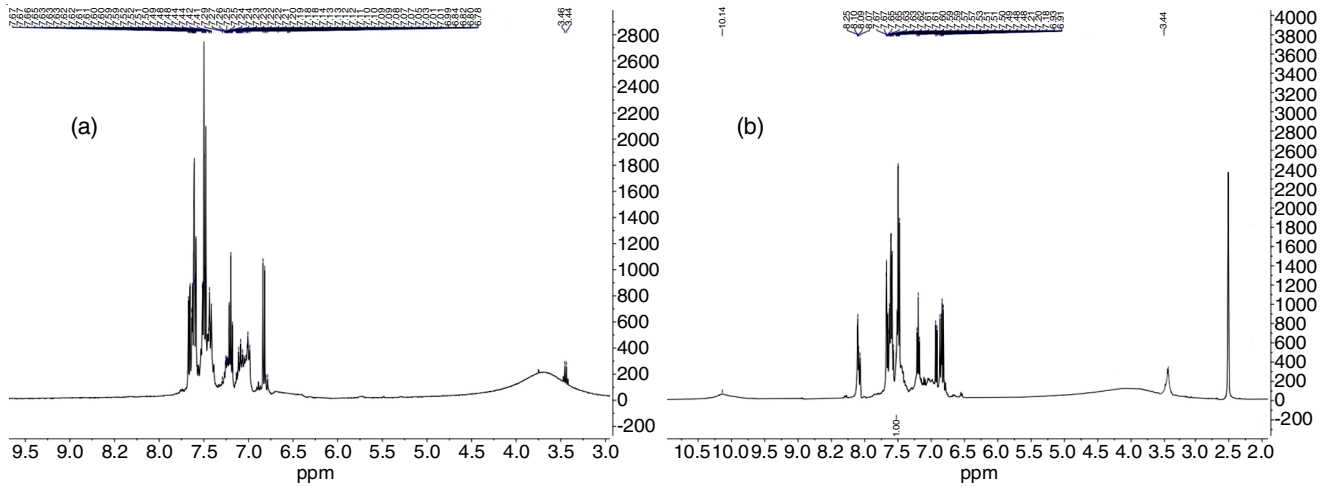


Fig. 3. ^{1}H NMR spectrum of the (a) ligand (NPhIATP) and (b) $RTeCl_3$·NPhIATP (**9d**)

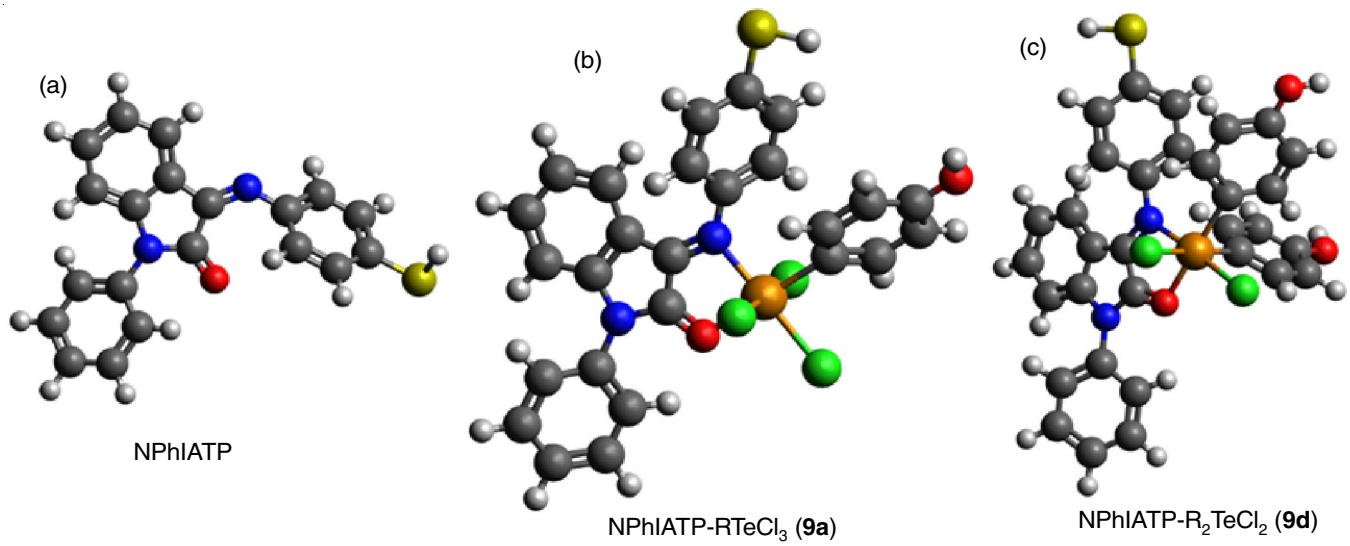


Fig. 4. (a) Optimized structure of (a) NPhIATP (b) complex **9a** (c) complex **9d**; Colour code: blue-N; red-O; grey-C; white-H; green- Cl; yellow-Te

TABLE-2
THE CALCULATED BOND LENGTHS (Å) AND SELECTED BOND ANGELS (°) OF SCHIFF BASE LIGAND AND ORGANOTELLURIUM(IV) COMPLEXES

Compound	C=N	C=O	Te-N (azomethine)	Te-O (carbonyl)
NPhIATP	1.294	1.221	–	–
9a	1.298	1.229	2.062	2.015
9d	1.305	1.233	2.065	2.044
Compound **9a**				
Atom connectivity	Bond angles (°)	Atom connectivity	Bond angles (°)	
Cl-Te-Cl	91.6228	O-Te-Cl	96.8298	
Cl-Te-Cl	178.4149	N-Te-Cl	178.9796	
C-Te-Cl	90.4950	C-Te-Cl	91.0639	
O-Te-Cl	88.7987	O-Te-Cl	88.8875	
N-Te-Cl	89.3703	N-Te-Cl	90.7213	
Cl-Te-Cl	88.2795	O-Te-C	179.9744	
C-Te-Cl	83.1284	N-Te-C	97.0999	
N-Te-O	82.9410			

mainly on metal with less contribution of rings. Various quantum chemical parameters [46,47] such as hardness (η), electronegativity (χ), softness (S), chemical potential (Pi) and electrophilicity index (ω) are obtained from the energy values of HOMO and LUMO listed in Table-3.

TABLE-3
THEORETICAL CALCULATED QUANTUM PARAMETERS OF THE LIGAND, **9a** AND **9d**

Parameters	Ligand (NPhIATP)	**9a**	**9d**
E_{HOMO} (eV)	-6.828	-3.599	-3.550
E_{LUMO} (eV)	-2.937	-0.278	-0.255
ΔE (eV)	3.891	3.321	3.295
IE (eV)	6.828	3.599	3.550
χ (eV)	4.8825	1.9385	1.9025
η (eV)	1.9455	1.6605	1.6475
S $(eV)^{-1}$	0.2570	0.3011	0.3034
ω (eV)	6.1265	1.1314	1.0898
Pi	-4.8825	-1.9385	-1.9025

Molecular docking studies: Autodock vina tools were used to determine the protein-ligand interactions [48,49] between receptor of proteins and drugs. The molecular docking analysis

is used to stimulate the biological features of drugs with optimized conformations of proteins. Molecular docking study has been carried out between ligand (NPhIATP) and two receptor proteins of *E. coli* (3t88) and *S. aureus* (3ty7). The 3D interactions between ligand and proteins are shown in Fig. 5, which confirm the mode of interactions between ligand and various amino acids residue *via* hydrogen bonding in the docking pocket. Many hydrophobic non-polar interactions were also present between aromatic carbons of ligand and amino acid residues. The estimated value of binding energy of affinity (Kcal/mol), drug score and interaction surface area were determined. More negative value of binding energy represents the more efficient interactions which follows the order:

E. coli (3t88) > *S. aureus* (3ty7)

The estimated binding energies for ligand showed stronger affinity towards the proteins and can be used as antimicrobial drug. For receptor *E. coli* (3t88), leucine (Leu198) residue showed hydrogen bonding (bond length 3.12 Å) with ligand. The binding energy with value -8.5 kcal/mol was found to be higher than proteins of *S. aureus* (3ty7). The drug score and surface area were found to be 0.37 and 687.57 $Å^2$.

For receptor *S. aureus* (3ty7), the value of estimated binding energy, drug score and interacting surface area were found to be -7.8 kcal mol^{-1}, 0.55 and 811.31 $Å^2$, respectively. Ligand forms hydrogen bond with leucine (Ile 244) and phenylalanine (Phe 235) amino acid residue with bond lengths 2.97 and 3.04 Å, respectively.

Antimicrobial studies: The newly synthesized ligand (NPhIATP) and organotellurium(IV) complexes (**9a-f**) were

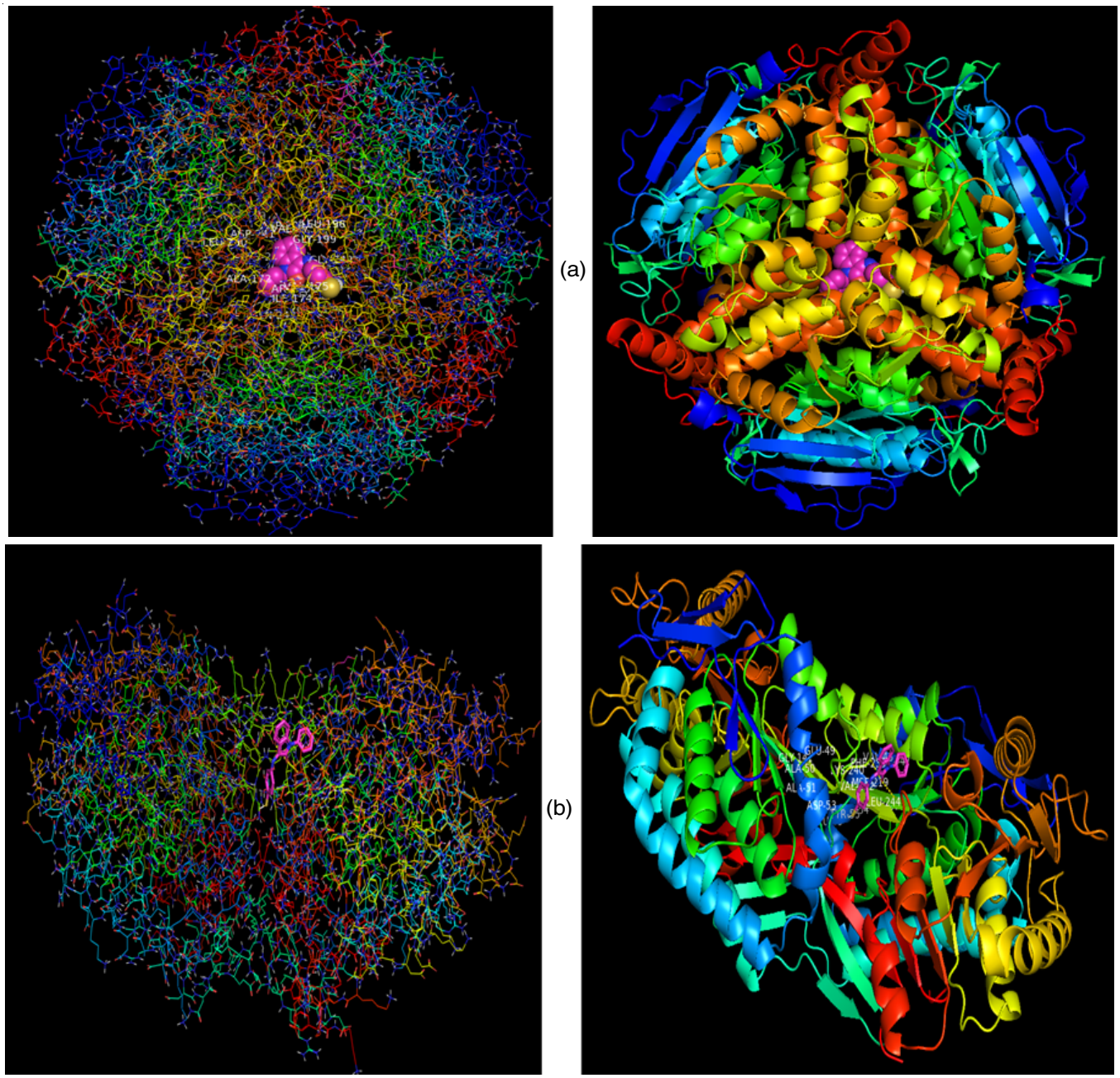


Fig. 5. 3D plot of interactions of (a) NPhIATP with *E. coli* (3t88) and (b) NPhIATP with *S. aureus* (3ty7)

TABLE-4
ANTIBACTERIAL AND ANTIFUNGAL ACTIVITY OF LIGAND (NPhIATP) AND COMPLEXES (**9a-f**)

Compound	Antibacterial activity (diameter in cm)				Antifungal activity (diameter in cm)			
	Bacillus cereus	*Xanthomonas campestris*	*Staphylococcus aureus*	*Escherichia coli*	*Fusarium oxysporum*	*Macrophomina phaseolina*	*Rhizoctonia solani*	*Candida albicans*
NPhIATP	1.2	1.5	1.4	1.4	1.1	0.8	1.2	0.9
9a	2.8	2.6	2.3	1.8	1.3	2.4	2.6	2.9
9b	2.6	2.2	2.0	2.0	1.8	1.1	1.6	3.1
9c	3.2	3.4	2.5	2.5	2.6	1.9	2.8	2.8
9d	1.4	3.1	2.1	2.3	2.2	2.9	3.1	3.4
9e	1.6	1.9	2.3	2.1	2.8	1.8	2.6	3.2
9f	1.2	3.0	1.8	1.7	1.2	1.3	2.3	2.1
Tetracycline	1.8	1.4	1.7	0.9	–	–	–	–
Cycloheximide	–	–	–	–	1.5	1.0	1.2	1.3

evaluated for their antibacterial activity against bacterial (*B. cereus*, *X. campestris*, *E. coli* and *S. aureus*) and antifungal activity against fungal strains (*F. oxysporum*, *C. albicans*, *R. solani*, *M. phaseolina*). The growth inhibition zones of all compounds were measured and results are shown in Table-4. All the compounds exhibited good activity against all bacteria. Schiff base (NPhIATP) was effective against with different bacterial strains with zone of inhibition of 1.2-1.5 cm, whereas complexes **9c**, **9d** and **9e** showed better activity against *E. coli* and *S. aureus* with inhibitory zones in range of 2.1-2.5 mm. Complex **9a** was highly effective against *B. cereus*, *X. campestris* and *S. aureus*. Complex **9d** show best activity whereas **9f** showed least effectiveness against fungi *C. albicans*. Complex **9c** was found to be most active against all the bacteria. Thus, it was concluded that on complexation, antimicrobial activity enhanced, explained on the basis of chelation theory. Due to chelation, polarity on the tellurium(IV) ion get reduced and its lipophilic character increases. Also, the biological activities of the complexes are influenced by steric factor, nature of ligand, donor atoms, size of metal ion, geometry and coordination sites. The antifungal activity of compounds ranged from 1.1-3.1 mm. Schiff base ligand show moderate activity against *M. phaseolina* and *C. albicans*. All other compounds showed good activity against all the studied fungi.

Conclusion

In this work, six organotellurium(IV) complexes (**9a-f**) of Schiff base (NPhIATP) have been synthesized and characterized by molar conductance, FT-IR, mass spectrometry, UV-Visible, elemental analyses, ^{1}H & ^{13}C NMR spectroscopy. The geometrical optimization and spectroscopic techniques purposed the distorted octahedral geometry of the complexes. The antimicrobial activity of these organotellurium(IV) complexes were compared with ligand and found to be more active. Molecular docking results were relevant to expermiental results and ligand can act as good antimicrobial agent against reported microorganisms. Among all the complexes, **9c** shows best the antimicrobial activity against reported bacterial and fungal strains.

ACKNOWLEDGEMENTS

Authors are grateful to UGC for Senior research fellowship. We are thankful to CIL, M.D. University, Rohtak for IR, UV and CHN analyses, Guru Jambeshwar University, Hisar for NMR spectroscopy, IIT Ropar for Mass spectra and Haryana Agriculture University, Hisar, India for antimicrobial studies.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

REFERENCES

1. P.G. Cozzi, *Chem. Soc. Rev.*, **33**, 410 (2004); https://doi.org/10.1039/B307853C
2. M. Bouhdada, M. El Amane and N. El Hamzaoui, *Inorg. Chem. Commun.*, **101**, 32 (2019); https://doi.org/10.1016/j.inoche.2019.01.005
3. B.K. Singh, A. Prakash, H.K. Rajour, N. Bhojak and D. Adhikari, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, **76**, 376 (2010); https://doi.org/10.1016/j.saa.2010.03.031
4. B. Iftikhar, K. Javed, M.S.U. Khan, Z. Akhter, B. Mirza and V. Mckee, *J. Mol. Struct.*, **1155**, 337 (2018); https://doi.org/10.1016/j.molstruc.2017.11.022
5. W.H. Mahmoud, R.G. Deghadi and G.G. Mohamed, *Appl. Organomet. Chem.*, **30**, 221 (2016); https://doi.org/10.1002/aoc.3420
6. A.A. Bekhit, H.T.Y. Fahmy, S.A.F. Rostom and A.M. Baraka, *Eur. J. Med. Chem.*, **38**, 27 (2003); https://doi.org/10.1016/S0223-5234(02)00009-0
7. B.M. Sahoo, S.C. Dinda, B.V.V.R. Kumar, J. Panda and P. Brahmkshatriya, *Lett. Drug Des. Discov.*, **11**, 82 (2013); https://doi.org/10.2174/1570180813109990041
8. A. Bacchi, M. Carcelli, P. Pelagatti, G. Pelizzi, M.C. Rodriguez-Arguelles, D. Rogolino, C. Solinas and F. Zani, *J. Inorg. Biochem.*, **99**, 397 (2005); https://doi.org/10.1016/j.jinorgbio.2004.10.008
9. G. Saravanan, P. Pannerselvam and C.R. Prakash, *J. Adv. Pharm. Technol. Res.*, **1**, 320 (2010); https://doi.org/10.4103/0110-5558.72426
10. P. Panneerselvam, R.R. Nair, G. Vijayalakshmi, E.H. Subramanian and S.K. Sridhar, *Eur. J. Med. Chem.*, **40**, 225 (2005); https://doi.org/10.1016/j.ejmech.2004.09.003
11. Deepak, S. Chauhan, K.K. Verma and S. Garg, *Chem. Sci. Trans.*, **6**, 339 (2017); https://doi.org/10.7598/cst2017.1391
12. S.I. Al-Resayes, M. Shakir, A. Abbasi, K.M.Y. Amin and A. Lateef, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, **93**, 86 (2012); https://doi.org/10.1016/j.saa.2012.02.099
13. S. Chauhan and S. Deepak, *Int. J. Chem. Sci.*, **14**, 269 (2016).
14. Deepak, S. Chauhan, K.K. Verma and S. Garg, *Chem. Sci. Trans.*, **6**, 448 (2017); https://doi.org/10.7598/cst2017.1394

15. S.M. Saadeh, *Arab. J. Chem.*, **6**, 191 (2013); https://doi.org/10.1016/j.arabjc.2010.10.002
16. G. Goyat, S. Garg and K.K. Verma, *Chem. Sci. Trans.*, **5**, 479 (2016); https://doi.org/10.7598/cst2016.1204
17. G. Goyat, A. Malik, S. Garg and K.K. Verma, *Int. J. Chem. Sci.*, **14**, 1498 (2016).
18. A. Kriza and C. Parnau, *Acta Chim. Slov.*, **48**, 445 (2001).
19. M. Verma, S.N. Pandeya, K.N. Singh and J.P. Stables, *Acta Pharm.*, **54**, 49 (2004).
20. S.N. Pandeya, D. Sriram, G. Nath and E. De Clercq, *Arzneimittel-Forschung Drug Res.*, **50**, 55 (2000); https://doi.org/10.1055/s-0031-1300164
21. G. Goyat, A. Malik, S. Garg and K.K. Verma, *J. Chem. Pharm. Res.*, **8**, 218 (2016).
22. A. Deepak, S. Chauhan, K.K. Verma and S. Garg, *Int. J. Chem. Sci.*, **15**, 182 (2017).
23. A. Malik, G. Goyat, K.K. Verma and S. Garg, *Int. J. Sci. Res. Sci. Eng. Technol.*, **4**, 763 (2018).
24. A. Weissberger, Technique of Organic Chemistry, Interscience Publishers, Inc., New York, vol. 7 (1955).
25. N. Strafford, Eds.: A.I. Vogel, Practical Organic Chemistry, Including Qualitative Organic Analysis, Longmans, Green and Co.: London, New York, Toronto, Eds.: 3, p. 300 (1956).
26. G.T. Morgan and H.D.K. Drew, *J. Chem. Soc. Trans.*, **127**, 2307 (1925); https://doi.org/10.1039/CT9252702307
27. J. Bergman, *Tetrahedron*, **28**, 3323 (1972); https://doi.org/10.1016/S0040-4020(01)93674-9
28. N. Petragnani and H.A. Stefani, *Org. Synth.*, **1**, 9 (2007).
29. B.L. Khandelwal, K. Kumar and K. Reina, *Synth. React. Inorg. Met. Chem.*, **11**, 65 (1981); https://doi.org/10.1080/00945718108059276
30. B.L. Khandelwal, K. Kumar and F.J. Berry, *Inorg. Chim. Acta*, **47**, 135 (1981); https://doi.org/10.1016/S0020-1693(00)89319-6
31. N.N. Greenwood, B.P. Straughan and A.E. Wilson, *J. Chem. Soc. A Inorg. Phys. Ther.*, **4**, 2209 (1968); https://doi.org/10.1039/j19680002209
32. W.J. Geary, *Coord. Chem. Rev.*, **7**, 81 (1971); https://doi.org/10.1016/S0010-8545(00)80009-0
33. A. Apelblat, *J. Solution Chem.*, **40**, 1234 (2011); https://doi.org/10.1007/s10953-011-9718-y
34. A. Hassan and M.A. Khalifa, *J. Chem. Soc. Pak.*, **18**, 115 (1996).
35. S.A. Patil, S.N. Unki, A.D. Kulkarni, V.H. Naik, U. Kamble and P.S. Badami, *J. Coord. Chem.*, **64**, 323 (2011); https://doi.org/10.1080/00958972.2010.541240
36. J.E. Kovacic, *Spectrochim. Acta A*, **23**, 183 (1967); https://doi.org/10.1016/0584-8539(67)80219-8
37. R. Ramesh and S. Maheswaran, *J. Inorg. Biochem.*, **96**, 457 (2003); https://doi.org/10.1016/S0162-0134(03)00237-X
38. A.K. El-Sawaf, F. El-Essawy, A.A. Nassar and E.S.A. El-Samanody, *J. Mol. Struct.*, **1157**, 381 (2018); https://doi.org/10.1016/j.molstruc.2017.12.075
39. R.M. Issa, A.M. Khedr and H.F. Rizk, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, **62**, 621 (2005); https://doi.org/10.1016/j.saa.2005.01.026
40. V.V. Raju, K.P. Balasubramanian, C. Jayabalakrishnan and V. Chinnusamy, *Nat. Sci.*, **3**, 542 (2011).
41. O.S. Oguntoye, A.A. Hamid, G.S. Iloka, S.O. Bodede, S.O. Owalude and A.C. Tella, *J. Appl. Sci. Environ. Manag.*, **20**, 653 (2016); https://doi.org/10.4314/jasem.v20i3.20
42. A. Jarrahpour, D. Khalili, E. De Clercq, C. Salmi and J.M. Brunel, *Molecules*, **12**, 1720 (2007); https://doi.org/10.3390/12081720
43. H. Pervez, Z.H. Chohan, M. Ramzan, F.U.H. Nasim and K.M. Khan, *J. Enzyme Inhib. Med. Chem.*, **24**, 437 (2009); https://doi.org/10.1080/14756360802188420
44. D. Sinha, A.K. Tiwari, S. Singh, G. Shukla, P. Mishra, H. Chandra and A.K. Mishra, *Eur. J. Med. Chem.*, **43**, 160 (2008); https://doi.org/10.1016/j.ejmech.2007.03.022
45. V.R. Chandrasekhar, K. Mookkandi Palsamy, R. Lokesh and D.T. Thangadurai, *Appl. Organomet. Chem.*, **33**, e4753 (2018); https://doi.org/10.1002/aoc.4753
46. A.Z. El-Sonbati, M.A. Diab, G.G. Mohamed, M.A. Saad, S.M. Morgan and S.E.A. El-Sawy, *Appl. Organomet. Chem.*, **33**, 1 (2019); https://doi.org/10.1002/aoc.4973
47. T. Abbaz, A. Bendjeddou and D. Villemin, *Int. J. Adv. Sci. Eng. Technol.*, **5**, 5150 (2018).
48. W.H. Mahmoud, N.F. Mahmoud and G.G. Mohamed, *J. Organomet. Chem.*, **848**, 288 (2017); https://doi.org/10.1016/j.jorganchem.2017.08.001
49. W.H. Mahmoud, G.G. Mohamed and A.M. Refat, *Appl. Organomet. Chem.*, **31**, e3753 (2017); https://doi.org/10.1002/aoc.3753