

FULL PAPER

Synthesis, DFT Calculation and Biological Activity of Some Organotellurium Compounds Containing Azomethine Group

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Article history: Received: 24 July 2018; revised: 20 July 2019; accepted: 11 October 2019. Available online: 26 December 2019. DOI: <http://dx.doi.org/10.17807/orbital.v11i7.1211>

Abstract:

The reaction of (4-amino-2,3-dichlorophenyl)mercury (II) chloride with 3,4-dihydroxy benzaldehyde produce the organomercury compound **1** in 82% yield. Tellurated of **1** with tellurium (IV) tetrabromide gave the tellurium (IV) tribromide Schiff base compound **2**. The reaction between **1** and **2** gave the diaryltelluride dibromide compound **4**. Reduction of **2** and **4** by hydrazine hydrate gave diaryl ditelluride **3** and diaryl telluride **5** respectively in 53% and 61% yields. All new compounds were characterized by FT-IR, NMR and mass spectroscopy. The geometry optimization of molecular structure and energies was calculated using density functional theory by Material studio-DMol3 program. The synthesized compounds were screened for their antibacterial activity against *Escherichia coli*, *Pseudomonas* spp., *Klebsiella pneumonia*, *Proteus* and *Staphylococcus aureus*. Additionally, the compounds were tested as antioxidant activity by DPPH(1,1-Diphenyl-2-picryl-hydrazyl) assay method. The compounds exhibited its have antibacterial and antioxidant activity, and the compounds **2** and **4** gave higher activity than other compounds.

Keywords: antibacterial; antioxidant; computational study; organotellurium; Schiff bases

1. Introduction

Organotellurium compounds are versatile and useful organometallic due to their excellent nucleophilic reactivity, importance in synthetic organic chemistry and biological activity [1-5]. In recent decades, there has been a growing interest in studying the organotellurium compounds containing azomethine group due to high stability and various application of these compounds [6,7]. Synthesis tellurated Schiff bases by reacting Schiff bases with tellurium tetrabromide were failed and leading to ionic products [8], therefore, it can be prepared by treating the tellurated aldehydes with amines or treating tellurated amines with aldehydes or ketones [9] or by transmetallation reaction of mercurated Schiff base with tellurium tetrabromide [10-12]. Organotellurium compounds were found to have potent antioxidant activity, potent caspase and cathepsin inhibitors, anticancer, antitumor and pharmaceutical agents [13-17]. Also, it have potent immunomodulators (both in *vitro* and *vivo*)

with a variety of potential therapeutic application, for example, AS101 [ammonium trichloro (dioxoethylene-O, O)tellurate] and SAS [octa-O-bis-(R, R)-tartarate ditellurane] are effective in the treatment of AIDS and cancer[18-20].

Singh and McWhinnie [21] prepared (4-substituted-2-(phenyliminomethyl)phenyl) tellurium tribromide by reacting (4-substituted-2-(phenyliminomethyl) phenyl) mercuric chloride with tellurium tetrabromide which in turn reduced to the corresponding ditellurides by hydrazine hydrate. A range of novel chiral tellurium compounds having an azomethine group in ortho-position of tellurium atom were prepared by reaction of bis(2-formyl phenyl)telluride and 2-(butyl-telluro)benzaldehyde with chiral amines (*R*)-(+)-(1-phenylethylamine) and (1*R*,2*S*)-(-)-norephedrine, respectively [22].

Recently, number of publications reported the synthesis of series of organotellurium compounds containing azomethine group. Al-Fregi *et al.* [23] synthesized tellurated Schiff base bis[2-(3-

nitrobenzyl- ideneamino)-5-nitrophenyl] telluride and used as a ligand for metal complexes of Mn(II), Co(II) and Ni(II) ions. In our previous work [24] a series of tellurated Schiff bases were synthesized with formula ArTeBr_3 and Ar_2Te (where Ar = [2-(3,4-dihydroxy benzylideneamino)-5-sulfamoylphenyl] and [2-(3,4-dihydroxy benzylideneamino)-5-acetyl phenyl] which showed effectiveness as antioxidant and inhibition ability against tumor cell.

The aim of the present work is to synthesis some new organomercury and organotellurium containing azomethine group and characterized by FT- IR., ^1H NMR, ^{13}C NMR and mass spectra. In addition to studying biological activity of these compounds as antibacterial and antioxidant as well as study the molecular structure and energies by density faction theory (DFT) calculations, and then put a relationship between experimental results with theoretical calculations.

2. Results and Discussion

2.1. Synthesis

The present work describes the synthesis of new mercurated and tellurated compounds containing azomethine group. The reaction of (4-amino-2,3-dichlorophenyl) mercury(II) chloride with 3,4-dihydroxybenzaldehyde produce the new organomercury compound **1**. Tellurated of **1** by tellurium tetrabromide gave ortho- tellurated compounds **2**. The reaction compound **2** with **1** gave diaryl dibromidetelluride **4**. Reduction **2** and **4** compounds by hydrazine hydrate gave diaryl ditelluride **3** and diaryl telluride **5** respectively, as shown in Scheme 1. The structures of the synthesized compounds were assigned by the IR, ^1H and ^{13}C NMR and mass spectra. IR spectra for all compounds **1-5** showed a broad strong bands in the rang $3435\text{-}3491\text{ cm}^{-1}$ due to $\nu(\text{O-H})$ and a band at $1622\text{-}1635\text{ cm}^{-1}$ range can be attributed to $\text{C}=\text{C}$ aromatic. IR spectra confirm the presence of the azomethine group ($-\text{C}=\text{N}-$) stretching vibration with a sharp band at around $1571\text{-}1596\text{ cm}^{-1}$. The ^1H NMR spectra of studied compounds **1-5** showed all the expected protons with proper intensity ratio. It is worthy to note that the protons of Ar-OH resonate as a singlet signal between 9.18-9.45 ppm and it gave other evidence for forming azomethine group ($-\text{CH}=\text{N}-$) by showing a singlet signal within the range 7.95-

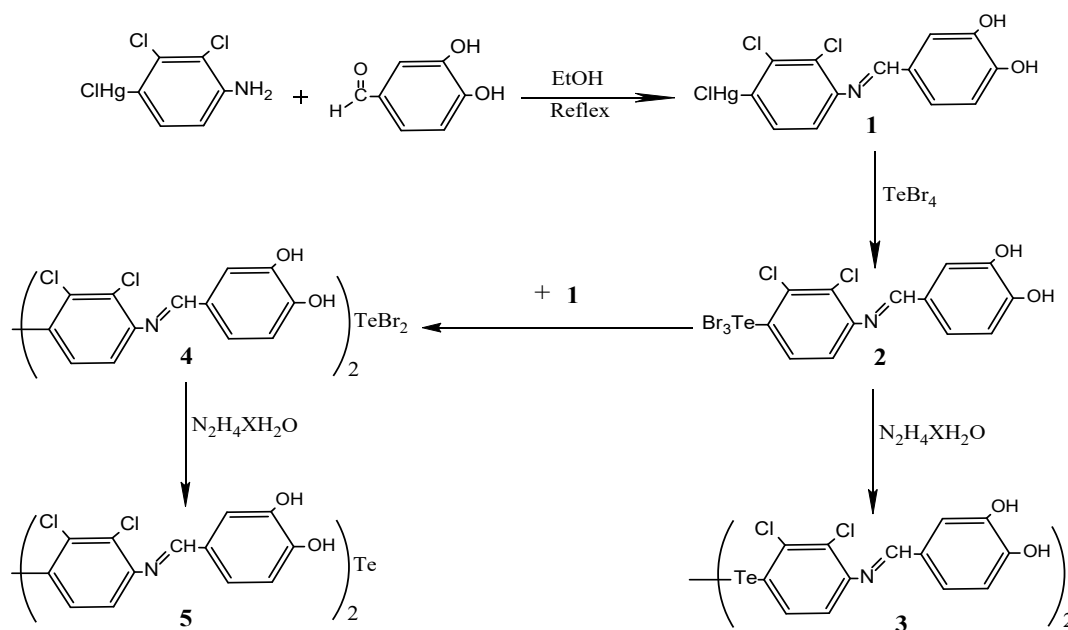
8.55 ppm, these values are in agreement with previously reported data [25]. The aromatic protons appeared as a multiplet signals within the range 6.55-7.89 ppm. ^{13}C NMR spectra of compounds **3** and **5** showed a low field signal at 162.03 and 161.61 ppm which is attributed to an aromatic carbon atom which is attached with the nitrogen atom ($\text{CH}=\text{N}-\text{C}$), while azomethine carbon atom appeared at 159.46 and 157.22 ppm [11]. Two signals at 146.35 and 142.75 ppm for compound **3** and 146.24 and 144.36 ppm for compound **5** can be assigned to aromatic carbon atoms which are attached with oxygen atoms, while the signals at 133.55, 129.89, 124.76 and 119.51 ppm for compound **3** and signals 134.05, 130.44, 123.07 and 117.37 ppm for compound **5** can be attributed to aromatic carbon atoms. Mass spectra of the synthesized compounds confirmed the correct structure by exhibited the peak of the molecular ion.

2.2. Computational study

The geometry optimization of the molecular structure of molecules **1-5** represented in Figure1 and structural parameters which are bonds lengths and angles are listed in Table 1. As shown in this table, there are slight changes in the bond lengths and angles of compounds indicate the presence of conjugation which causes of the electrostatic attraction between atoms, and this leads to redistribution of the electron cloud in the compounds when the replacing the H-C-Ph(ring) atom by different substituted (Cl-Hg, TeBr_3 , Te_2 , TeBr_2 , Te). The substitutes in the compounds can coordinate to the carbon ring. In compound **1** the distance between $[\text{d}(\text{Hg}-\text{C}) = 2.237\text{ \AA}]$, compound **2** $[\text{d}(\text{Te}-\text{C}) = 2.165\text{ \AA}]$, compound **3** $[\text{d}(\text{Te}-\text{C}) = 2.177\text{ \AA}]$, compound **4** $[\text{d}(\text{Te}-\text{C}) = 2.183\text{ \AA}]$, and compound **5** $[\text{d}(\text{Te}-\text{C}) = 2.157\text{ \AA}]$. The distance between $[\text{d}(\text{Te}-\text{C})]$ in compound **5** is shorter than in compounds **2**, **3** and **4**, due to the existence of π -conjugation [26]. The bond would have resonance character between a double and a single bond which found in compound **5** and this lead to the greater extension of the whole π -conjugation in the case of compound **5** as molecular system. On the other hand, in the compound **1**, each mercury atom is linearly coordinated to a chloride and a carbon atom (angle C-Hg-Cl is 177.77°) which is fully characterized structurally. The electron lone pair

around tellurium atom should be stereochemically active according to VSEPR (Valence Shell Electron Pair Repulsion) theory, therefore the geometry of tellurium(II) on compounds **3** and **5** is related to the distorted pseudo-tetrahedral (angles C-Te-Te=99.94°, 98.701° ; C-Te-

C=95.89°). While the tellurium (IV) on compounds **2** and **4** the angles C-Te-Br=97.50°, 88.67°, 88.68°; C-Te-C= 101.29°, then they are significantly lower than the putative value of 120° for trigonal bipyramidal, so it is expected to have distorted trigonal bipyramidal geometry [27].



Scheme 1. Preparation of organotellurium compounds.

The total energies, the HOMO, LUMO and energy band gap (ΔE) calculation have been investigated after total optimization and the data summarized in Table 2. It can be seen the total energy determines the occurrence or non-occurrence of chemical reactions and stereospecific paths in intra- and intermolecular processes. The total energy of the system composed of the internal, potential, and kinetic energy [28], the total energy (absolute values) for compounds are $1 > 3 > 2 > 4 > 5$. The eigenvalues of LUMO and HOMO and their energy gap reflect the chemical activity of the molecule and stability of structures. As well as the energy of the HOMO is directly related to the ionization potential, while LUMO energy is directly related to the electron affinity [29]. A compound with a small LUMO-HOMO energy gap can be associated with a high chemical reactivity, low kinetic stability and more polarizable this termed as soft molecule, so we expect the compound **2** has high biological activity compare with other compounds, while the compound with a large energy gap implies higher stability and lower chemical reactivity, so the

compound **1** is more stable compare with other compounds [30,31]. These results are in good agreement with the results that obtained from biological activity.

The dipole moment (μ in Debye) is another important electronic parameter used to describe the polarity of the molecule. This parameter helps in understanding of interaction between atoms, in the same or different molecules dipole moment, increases with an increase in electronegativity of atoms. Chemical reactivity usually increases with an increase in dipole moment and it is attractive for the interaction with other systems form complexes. From Table 2, the dipole moment has maximum values for compounds **2** and **4** compared with compounds **1**, **3** and **5**. The high dipole moment may make the compound **4** attract other systems to interact, to form complexes, and to indicate highly polar molecules, because the compound **2** and **4** have **Br** atoms and one **Te** atom, which led to increasing the chemical reactivity and reverse the high electronegativity. [32, 33]. This is support our experimental data of biological activity.

Table 1. Some of the structural properties of the studied molecules.

| Bonds length (Å) | Molecule no. | | | | |
|-------------------|--------------|------------------------|------------------------------------|------------------------------------|------------------------------------|
| | 1 | 2 | 3 | 4 | 5 |
| Cl-Hg | 2.432 | ---- | ---- | ---- | ---- |
| Hg-C | 2.237 | ---- | ---- | ---- | ---- |
| C-Cl | 1.758 | 1.741 | 1.734 | 1.731 | 1.742 |
| C-Cl | 1.733 | 1.727 | 1.746 | 1.735 | 1.735 |
| C-N | 1.391 | 1.387 | 1.395 | 1.385 | 1.391 |
| N=C | 1.289 | 1.290 | 1.285 | 1.284 | 1.284 |
| C-H | 1.107 | 1.107 | 1.101 | 1.101 | 1.100 |
| C-C | 1.456 | 1.454 | | | 1.398 |
| C-O | 1.361 | 1.360 | 1.381 | 1.380 | 1.381 |
| O-H | 0.977 | 0.977 | 0.972 | 0.972 | 0.972 |
| C-O | 1.381 | 1.380 | 1.360 | 1.354 | 1.361 |
| O-H | 0.972 | 0.972 | 0.977 | 0.977 | 0.977 |
| Br-Te | ---- | 2.702 | ---- | ---- | ---- |
| Br-Te | ---- | 2.583 | ---- | ---- | ---- |
| Br-Te | ---- | 2.706 | ---- | ---- | ---- |
| Te-Te | ---- | ---- | 2.753 | ---- | ---- |
| Te-Br | ---- | ---- | ---- | 2.758 | ---- |
| Te-Br | ---- | ---- | ---- | 2.719 | ---- |
| Te-C | ---- | 2.165 | ---- | ---- | ---- |
| Te-C | ---- | ---- | 2.177 | ---- | ---- |
| Te-C | ---- | ---- | ---- | 2.183 | ---- |
| Te-C | ---- | ---- | ---- | ---- | 2.158 |
| Angles (°) | | | | | |
| Cl-Hg-C | 177.77 | ---- | ---- | ---- | ---- |
| Br-Te-C | ---- | 97.50 , 88.67 88.68 | ---- | 89.63 , 92.79 87.10 , 96.20 | ---- |
| Te-C-C | ---- | 124.26 114.99 | 123.43 , 117.79 122.76 , 113.35 | 127.48 , 112.96 121.31 , 118.14 | 120.87 , 120.62 119.05 , 122.49 |
| C-N=C | 120.13 | 121.21 | 126.02 , 124.54 | 128.16 , 127.70 | 125.94 , 126.77 |
| Te-Te-C | ---- | ---- | 99.94 , 98.701 | ---- | ---- |
| C-Te-C | ---- | ---- | ---- | 101.29 | 95.89 |

Table 2. The Total Energy, Dipole moment (μ), E_{HOMO} , E_{LUMO} , Energy Gap (eV).

| Comp. No. | Total energy (Ha.) | μ Debye | E_{HOMO} eV | E_{LUMO} eV | Energy Gap eV |
|-----------|--------------------|-------------|----------------------|----------------------|---------------|
| 1 | -20497.714 | 3.987 | -5.589 | -2.878 | 2.711 |
| 2 | -15960.295 | 7.465 | -5.819 | -4.222 | 1.597 |
| 3 | -16477.492 | 2.762 | -5.005 | -2.606 | 2.399 |
| 4 | -15011.319 | 8.920 | -5.576 | -2.920 | 2.656 |
| 5 | -9864.6186 | 1.920 | -4.614 | -2.650 | 1.964 |

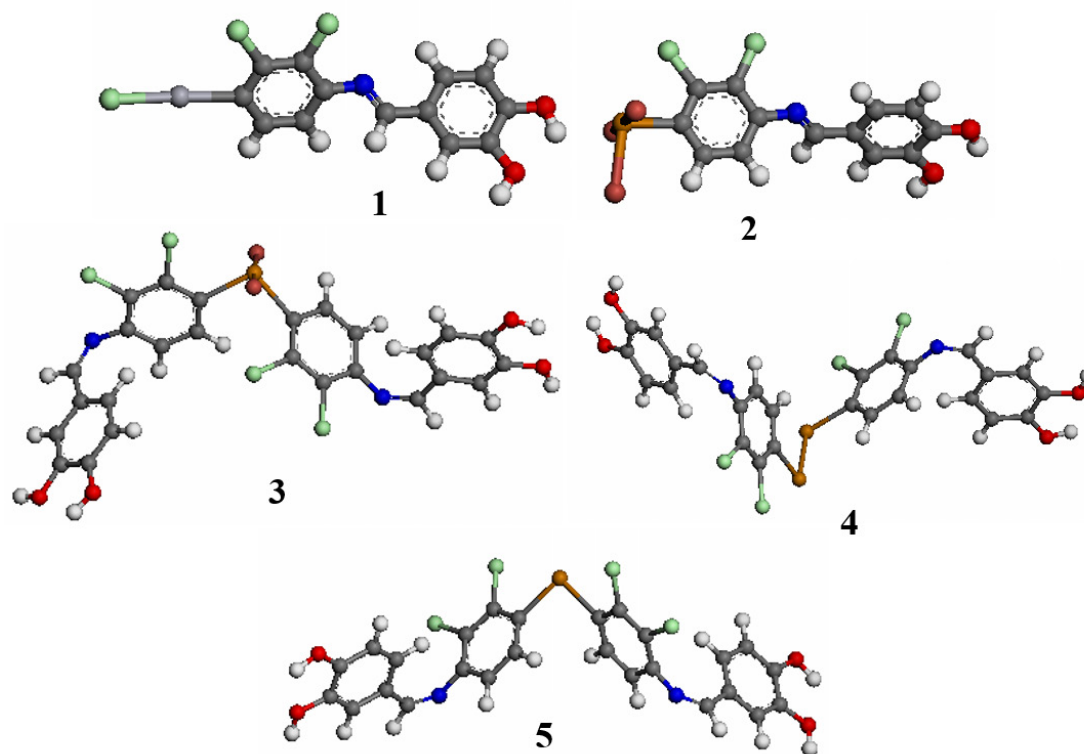


Figure 1. Optimization geometries structures of the studied molecules.

2.3. Antibacterial activity

The synthesized compounds have been screened for their *in vitro* antibacterial activities, using the paper disc-agar diffusion technique by measuring the inhibition zone in millimeter. The antibiotic ampicillin was used as a control against bacteria. The antibacterial activity of the synthesized compounds was tested against four gram negative bacteria (*E.coli*, *Pseudomonas spp.*, *Klbsiella pneumonia*, *proteus*) and one gram positive bacteria (*Staphylococcus aureus*) at a concentration of 200 μ g/ml using DMSO as a solvent, which not effected the growth of microbes. Muller Hinton agar was used as culture media for antibacterial activity. The results of the antibacterial activity are shown in Table 3. All compounds exhibited activity against all the bacterial species. However, the compounds have

the highest activity against *E. coli*, *Pseudomonas spp.*, *Klbsiella pneumonia* but it showed a moderate activity against *Staphylococcus aureus* and *proteus*. It is worth noting that all compounds have activity against both gram positive and negative bacteria. Therefore, a plausible explanation of our results attributed to the chemical structure of the bacterial cells wall which provides important ligands for adherence and receptor sites for antibiotic and drugs. As could be seen from the inhibition zone values, Table 3 shows that the compounds **2** and **4** have higher activity, this may be due to presence the bromine and tellurium atoms as well as the tellurium atom has tetravalent, which increase the chemical reactivity and reverse the high electronegativity [32]. These facts are agreement with previous study performed in different concentrations [3].

Table 3. Antibacterial activity of studied compounds.

| Comp. No. | Diameter of inhibition zone in mm for different microbial species | | | | |
|------------|---|---------------------|-----------------------|---------------------|---------------------|
| | <i>E. coli</i> | <i>Pseudo. spp.</i> | <i>Klbs.pneumonia</i> | <i>Staph.aureus</i> | <i>Proteus spp.</i> |
| 1 | 0 | 15 | 18 | 10 | 8 |
| 2 | 40 | 15 | 14 | 16 | 8 |
| 3 | 28 | 15 | 10 | 13 | 10 |
| 4 | 40 | 16 | 19 | 10 | 8 |
| 5 | 28 | 15 | 0 | 10 | 0 |
| Ampicillin | 30 | 32 | 38 | 42 | 19 |

DMSO solvent is negative antibacterial.

2.4. Antioxidant activity

The DPPH assay method is depended on the reduction of 1,1-Diphenyl-2-picryl-hydrazyl molecule, a stable free radical. The DPPH with an odd electron gives a maximum absorption at 517 nm (purple colour). When antioxidants react with DPPH, which is a stable free radical, it is paired off in the presence of a hydrogen donor (e.g., a free radical-scavenging antioxidant) and is reduced to the DPPH-H. Consequently, the absorbance decreased from the DPPH. Radical to the DPPH-H form, results in decolorization (yellow colour) with respect to the number of electrons are captured [34]. The antioxidant activity of studied compounds **1-5** have been tested by using DPPH method, Figure 2 shows the absorbance curves of free radical DPPH with studied compounds against time. A lower absorbance at 517 nm indicates the antioxidant activity for these compounds.

The scavenging activity was calculated by using the following equation [35]:

$$\text{Scavenging\%} = \frac{[\text{Abs. of control} - \text{Ab. of test sample}]}{[\text{Abs. of control}]} \times 100$$

The values of scavenging activity and half-life time of proton donating (T_{IC50}) gathered in Table 4. From the results we have obtained, the order of effectiveness of compounds is follows: **2>4>5>3>1**. The antioxidant activity of studied compounds is due to presence of hydroxyl phenolic group, polyphenols are reported to have a higher antioxidant activity than monophenols because of the effective delocalization of an unpaired electron [36], it may be due to the specific properties of the tellurium atom, such as charges and radical stabilization [37], and the presence of vacant *d*-orbital as potent oxidizing agents [38]. The compounds **2** and **4** found have high antioxidant activity because of tellurium atom is tetravalent [39].

Table 4. Data of antioxidant activity for studied compounds.

| Comp. No. | Activity% | T_{IC50} (min) |
|-----------|-----------|------------------|
| 1 | 46.03 | 33.0 |
| 2 | 55.40 | 12.5 |
| 3 | 48.08 | 19.5 |
| 4 | 52.91 | 14.5 |
| 5 | 51.45 | 16.5 |

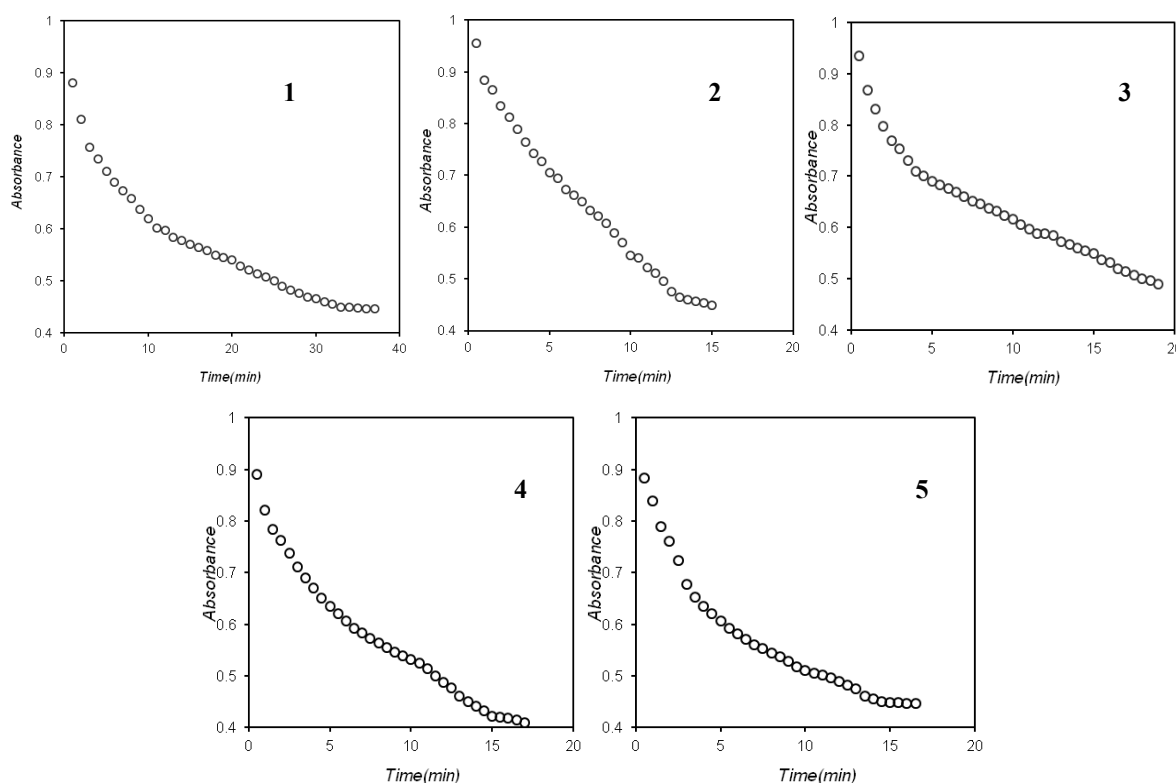


Figure 2. Reaction curves of DPPH radical with studied compounds in ethanol at 517 nm.

3. Material and Methods

3.1. Materials and Instruments

Melting points of compounds were determined by a thermo.Scientific (9100), Electro thermal Engineering LTD, UK. Infrared spectra were recorded as KBr discs using FT-IR spectrophotometer Shimadzu model IR.Affinity-1 in Chemistry department, Education for Pure sciences College, University of Basra, Iraq. ^1H and ^{13}C NMR spectra were obtained on Bruker 400 MHz spectrometer at the laboratory of Kashan University, Iran by using DMSO- d_6 as a solvent and the tetramethyl silane (TMS) as an internal reference. Mass spectra were recorded by using ESI Technique with HPLC-CQ Fleet/Thermo Scientific (NHRF) spectrometer at Helink international researches center, Athena, Greece.

3.2. Synthesis methods

(2,3-dichloro-4-(3,4-

dihydroxybenzylideneamino)phenyl)mercury(II) chloride 1: A mixture of (5.00 mmol, 1.98 g) of (4-amino-2,3-dichlorophenyl)mercury(II) chloride (which prepared according to literature[40]) and (5.00 mmol, 0.69 g) of 3,4-dihydroxybenzaldehyde in 30 mL of ethanol with 2-3 drops of sulfuric acid were refluxed with stirring for 2 hours. After cooling, the precipitate was collected by filtration and washed several times with ethanol. The solid product was twice recrystallized from a mixture of ethanol and benzene (3:2) to give a yellowish solid. Yield: 82%. m.p.: 176-178°C(dec.). FT-IR (KBr, ν , cm^{-1}): 3491 (OH), 3120(arom.CH), 2951 and 2901(aliph. CH), 1624 (C=C), 1582 (C=N). ^1H NMR (DMSO- d_6 , δ , ppm): 9.40 and 9.18 (s, 2H, OH), 8.42(s, 1H, -N=CH), 7.22-7.81 (m, 5H, Ar-H). MS (ESI, m/z (%)): 517[M^+ , 66.3].

(2,3-dichloro-4-(3,4-

dihydroxybenzylideneamino)phenyl)tellurium(IV)tribromide 2: A mixture of (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)mercury(II) chloride **1** (1.55 g, 3.00 mmol) and tellurium tetrabromide (1.34 g, 3.00 mmol) in 40 mL of 1,4-dioxane was refluxed for 6 hours under argon atmosphere. On cooling separated the complex of

dioxane and mercury (II) halide as white plates and removed by filtration. The filtrate was concentrated on the rotary evaporator. Evaporation was carried out to dryness and the residue was recrystallized (twice) from a mixture of methanol and dichloromethane (2:1) gave a brown solid crystal. Yield: 63%. m.p.: 213-215°C(dec.). FT-IR (KBr, ν , cm^{-1}): 3450 (OH), 3111(arom.CH), 2965 (aliph. CH), 1633 (C=C), 1571 (C=N). ^1H NMR (DMSO- d_6 , δ , ppm): 9.45 and 9.23 (s, 2H, OH), 8.37(s, 1H, -N=CH), 7.07-7.89 (m, 5H, Ar-H). MS (ESI, m/z (%)): 650[M^+ +1, 55.1].

Bis (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)

ditelluride 3: Hydrazine hydrate (0.76 g, 15.00 mmol) in 10 mL of ethanol was added very slowly to a refluxing solution of (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)tellurium(IV) tribromide **2** (1.29 g, 2.00 mmol) in 20 mL of ethanol. Each addition was accompanied by a vigorous evolution of nitrogen. On completing the addition, and no further nitrogen was evolved, the mixture was cooled and collected the precipitate by filtration, washed with methanol and dried in vacuum. Recrystallization from ethanol gave a dark reddish-brown solid, Yield: 53%. m.p.: 263-266°C(dec.). FT-IR (KBr, ν , cm^{-1}): 3443 (OH), 2917(aliph. CH), 1624 (C=C), 1580 (C=N). ^1H NMR (DMSO- d_6 , δ , ppm): 9.39(s, 1H, OH), 7.95 (s, 2H, -N=CH), 6.58-7.65 (m, 10H, Ar-H). ^{13}C NMR (DMSO- d_6 , δ , ppm): 162.03, 159.46, 146.35, 142.75, 133.55, 129.89, 124.76, 119.5. MS (ESI, m/z (%)): 818[M^+ +1, 45].

Bis (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)

tellurium(IV)dibromide 4: (2.00 mmol, 1.03 g) of 2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)mercury(II) chloride **1** and (2.00 mmol, 1.29 g) of (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)tellurium(IV) tribromide **2** in 30 mL of 1,4-dioxane were refluxed for 6 hours under argon atmosphere. The reaction mixture was filtered hot. The filtrate deposited a 2:1 complex of $\text{HgClBr}(\text{dioxane})_2$ as white plates upon cooling to room temperature. The white complex was filtered off. The filtrate was poured into 100 mL of ice - water, a brown precipitate was formed. The resulting

product was twice recrystallized from a mixture of methanol and dichloromethane (2:1) to afford yellowish brown solid, Yield: 64%. m.p.: 176-178°C(dec.). FT-IR (KBr, ν , cm^{-1}): 3438 (OH), 2951 and 2909(aliph. CH), 1623 (C=C), 1595 (C=N). ^1H NMR (DMSO- d_6 , δ , ppm): 9.31(s, 1H, OH), 8.55(s, 2H, -N=CH), 6.55-7.67 (m, 10H, Ar-H). MS (ESI, m/z (%)): 850[M⁺+1, 42].

Bis (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl)telluride

5: (2.0 mmol, 1.69 g) of Bis (2,3-dichloro-4-(3,4-dihydroxybenzylideneamino)phenyl) tellurium(IV) dibromide **4** was dissolved in 20 mL of ethanol under reflux. An ethanolic solution of hydrazine hydrate (1.00 g, 20.00 mmol) was added drop by drop until exit bubbles of nitrogen was stopped. The mixture was cooled and filtered off. The product was twice recrystallized from a mixture of ethanol and chloroform to give a yellowish orange solid Yield: 61%. m.p.: 246-249°C(dec.), FT-IR (KBr, ν , cm^{-1}): 3435 (OH), 3110 (arom.CH), 2904 (aliph. CH), 1624 (C=C), 1592 (C=N). ^1H NMR (DMSO- d_6 , δ , ppm): 9.28 (s, 1H, OH), 8.12(s, 2H, -N=CH), 6.90-7.78 (m, 10H, Ar-H). ^{13}C NMR (DMSO- d_6 , δ , ppm): 161.61, 157.22, 146.24, 144.36, 134.05, 130.44, 123.07, 117.37. MS (ESI, m/z (%)): 690[M⁺, 48.2].

3.3. Computational study

The computations of the geometries and energies of the synthesis compounds **1-5** were done using density functional theory (DFT) method, at the PBE level of theory along with standard DNP basis set [5, 12] and performed with Material studio-DMol3 Version 5.5 program [41]. And used Pc Pentium VI (CPU 3.1 GHz. Core i3, Ram 4 GB.). Work time was taken between 4-22 hours.

3.4. Antibacterial activity

The synthesized compounds were screened *invitro* for their antibacterial activity against *Escherichia coli*, *Pseudomonas spp.*, *Klasiella pneumonia*, *proteus* and *Staphylococcus aureus* using the paper disc-agar diffusion technique on Muller Hinton agar as a culture media for antibacterial activity[42]. The test compounds were dissolved in DMSO solvent and the

recommended a concentration of (200 $\mu\text{g/mL}$)[43] was used in the disc-agar diffusion technique. Antibiotic drug Ampicillin was used as a control. Petri plates containing 20 ml of Muller Hinton Agar were used for all the bacteria tested. Sterial Whatman no.1 filter paper disks (6mm in diameter) impregnated with the solution in DMSO of the test were placed on the petri plates. A paper disk impregnated with dimethylsulfoxide (DMSO) was used as negative control. The plates were incubated for 24h at 37°C. The inhibition zone diameters were measured in millimeters.

3.5. Antioxidant activity

The antioxidant activity performed by DPPH method [44]. 1×10^{-3} molar of both 1,1-Diphenyl-2-picryl-hydrazyl (DPPH) and studied compounds were prepared in Ethanol. The antioxidant activity of studied compounds was examined by mixing 0.5 mL from both DPPH and the studied compounds. The reaction was followed with time at 517 nm using 9200 UV/Vis. spectrophotometer at room temperature. The reaction was stopped after the T_{IC50} value (is the time at which the DPPH loses 50% of the original concentration).

4. Conclusions

In conclusion, the transmetallation reaction between mercury and tellurium atoms is a successful reaction to the preparation tellurated Schiff bases to give products in good yields. The synthesis organotellurium compounds containing azomethine group 2-5 was found to have antibacterial and antioxidant activity greater than organomercury, compound 1, addition to the Te(IV) orgnotellurium, 2 and 4 compounds have higher biological activity than Te(II) orgnotellurium, 3 and 5 compounds. These results are agreement with the results obtained from the theoretical studies, which includes the values of each LUMO-HOMO energy gap and dipole moment.

The author has a future plan of action for the development of the biological activity of 2 and 4 compounds and the experience of more types of biological activity in order to be able to use them as a drug).

Acknowledgments

The author is grateful to Chemistry department, College of education for pure sciences, University of Basrah, Iraq to support all facilities including laboratories and measurements of FT-IR spectra.

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