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RESEARCH ARTICLE

SYNTHESIS, CHARACTERIZATION, LIGAND PROPERTIES AND THEORETICAL STUDY OF SOME NEW ORGANIC TELLURIUM COMPOUNDS DRIVEN FROM INDOLE.

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Abstract

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New series of organotellurium compounds were prepared from reaction of 3-indolylmercurric chloride(**1**) with $TeBr_4$ in dioxin in mole ratio 1:1 to give indolyl tellurium tribromide(**2**) which reduced by hydrazine hydrate to give bis indolyl ditelluride(**4**). Reaction of 3-indolylmercuric chloride(**1**) with $TeBr_4$ in 2:1 mole ratio afforded bis indolyltellurium dibromide(**3**), reduction the later compound by hydrazine hydrate gave bis indolyltelluride(**5**), addition of thionyl chloride and iodine gave bis indolyltellurium dichloride(**6**) and bis indolyltellurium diiodide(**7**) respectively. Reaction of bis indolyltelluride(**5**) with palladium, platinum, and rhodium salts, respectively, afforded new complexes, i.e, bis{bis[3-(indolyl)] telluride}palladium(II) dichlorid (**8**) bis{bis[3-(indolyl)] telluride} platinum(II) dichloride (**9**) and bis{bis[3-(Indolyl)]telluride}rhodium(III) trichloride (**10**) in good yield respectively. All compounds were characterized by IR, Elemental analysis, Conductance measurements, ^{1}H-NMR, and Mass spectroscopy. Optimization structures and some of the selected structural parameters (charges and bond lengths) of the optimized geometries of all the prepared compounds were determined. The three-dimensional mapped isosurface of the electrostatic potential for selected compounds **2** and **5** were plotted.

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Introduction:-

Indole is a fused aromatic heterocyclic ring, consisting of a six-membered benzene ring fused to a five-membered nitrogen containing pyrrole ring.[1] Indole is also termed as a benzopyrrole because it derived by fusion of benzene and pyrrole rings through the 2-and 3-positions of the pyrrole nucleus.[2] Indole has a molecular formal C_8H_7N and is white crystal hygroscopic solid. It is possess unpleasant odor as a feces when impure while the pure indole has a pleasant as a jasmine odor. [3]

Indole is a classified as a π-excessive planar heterocyclic aromatic compound. it is isoelectronic with naphthalene with nitrogen heterocyclic atom donating two of the ten π-electrons . The aromaticity of the ring is fundamental to the success of many synthetic methods. [4] Indole undergoes electrophilic substitution mainly on position 3 which is the most reactive site for substitution due to a result which is explicable in terms of the contribution of resonance structures. The C3 position is estimated to be 10^{13} timers more reactive than benzene to electrophilic attack.[5] Indole react with mercuric chloride and mercuric acetate to give chloromercuri- and acetoxymercuri-derivatives respectively. Sodium chloride converts acetoxymercuri-derivatives to chloromercuri-derivatives. [6]

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Yudin *et al* [7] reported that reaction of 1-methylindole with mercuric chloride and mercuric acetate gave 1-methylindole-3-mercurichloride and 1-methyl-3-acetoxymercuri-indole, respectively. If the mercuration of unsubstituted N-H indole is carried out in acetic anhydride, acetylation of the NH group and the replacement of a hydrogen atom of the pyridine ring by an acetoxy mercury group take place simultaneously (at room temperature for 24 hr or boiling for 5-10 min) which in turn yield 1-acetyl -3-chloromercuriindole on treatment with sodium chloride. [8]

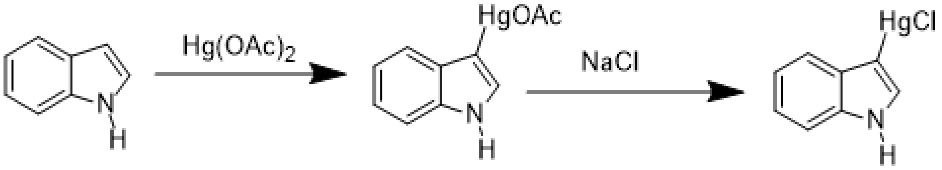
Mingoia [9] discovered that indole converts into 2,3-diacetoxy mercury indole by action of 2 equiv of mercuric acetate in ethanol **.** Treatment of indole with 2 moles of mercuric acetate in water or ethanol afforded in high yield a diacetoxy- mercuri derivative, which appeared to be 1,3-diacetoxy mercuriindole.

Large numbers of organotellurium compounds were prepared by transmetallation reaction of aromatic organomercuric chloride with $TeBr_4$ in dioxane in which the products depend on the mole ratio of Ar-HgCl to $TeBr_4$ if 1:1 gave Ar-$TeBr_3$ and 2:1 afford Ar_2TeBr_2which on reduction gave symmetrical tellurides.[10, 11]

In the present work, a series of new organotellurium compounds based on indole will be prepared via transmetallation reaction of 3-(indolyl) mercuric chloride with tellurium tetrabromide in 1:1 and 1:2 mole ratio, respectively. Furthermore, the ligand properties of bis[3-(indolyl)] telluride will be carried out with K_2PtCl_4, Na_2PdCl_4 and $RhCl_3.3H_2O$.

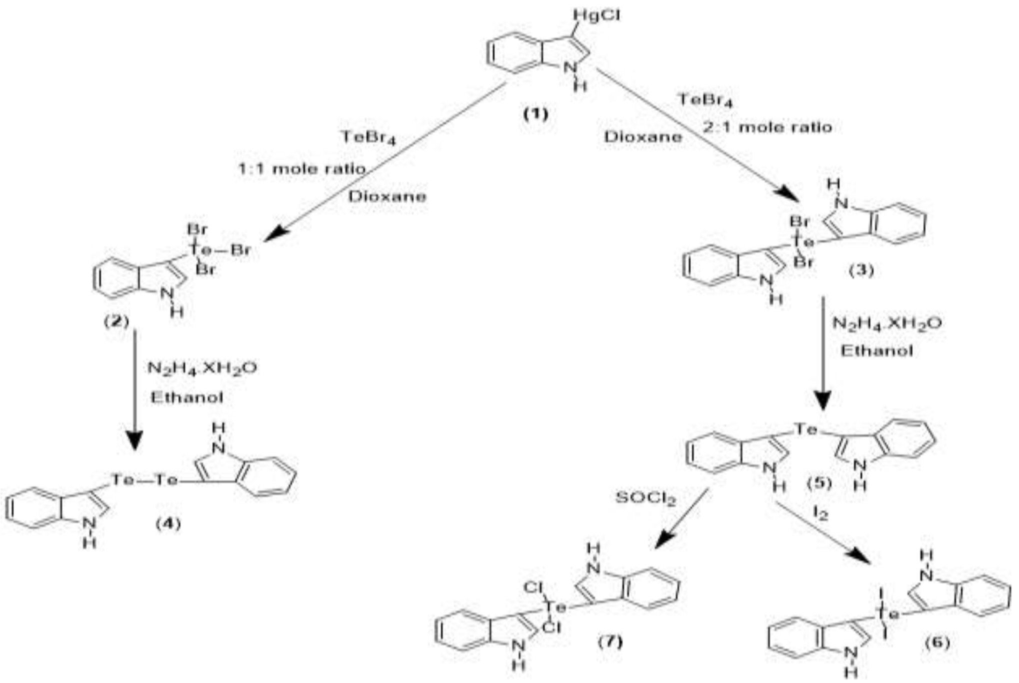
Results and disussion:-

The mercurated 3-(indolyl)mercuric chloride (**1**) was prepared by reacting of indole with mercuric acetate followed by addition of sodium chloride, *Scheme* 1. Compound **(1)** was obtained as white crystals in 77%.



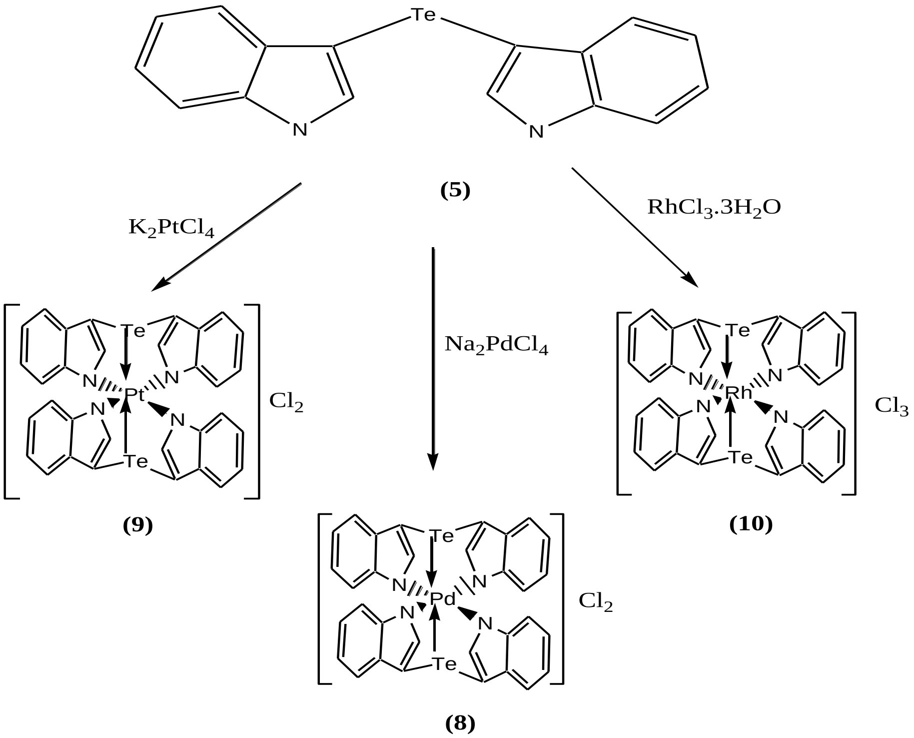
***Scheme* 1:-** Preparative method of compound (**1**)

Reaction of 3-(Indolyl) mercuric chloride (**1**) with tellurium tetrabromide in 1:1 mole ratio gave the 3-(indolyl) tellurium tribromide (**2**) as a light brown solid in 69 % yield , *Scheme* 2. When 3-(indolyl)mercuric chloride (**1**) was reacted with tellurium tetrabromide in 2:1 mole ratio, bis[3-(indolyl)]tellurium dibromide (**3**), was obtained as yellowish brown crystals in 71% yield, *Scheme* 2. Reduction of 3-(indolyl)tellurium tribromide (**2**) by ethanolic solution of hydrazine hydrate gave bis[3-(indolyl)] ditelluride (**4**) as dark red crystals in 55% yields , *Scheme* 2.
Bis[3-(indolyl)] telluride (**5**) was obtained as dark green solid in 59% yield by reduction of bis[3-(indolyl]tellurium dibromide (**3**) by solution of hydrazine hydrate in boiling ethanol. Bis[3-(indolyl)]tellurium dichloride (**6**) and bis[3-(indolyl)]tellurium diiodide (**7**) were prepared by reacting of bis[3-(indolyl)] telluride (**5**) with thionyl chloride and iodine respectively, *Scheme* 2. Compounds (**6** and **7**) were obtained as yellowish brown to brown solids in 82 and 85% yields, respectively.



***Scheme* 1:-** The preparative method for compounds (**1-7**).

In order to clarify the ligand properties of these new compounds to form complexes with metal salts, we selected bis[3-(indolyl)]telluride) (**5**) as a ligand with Na_2PdCl_4 , K_2PtCl_4, and $RhCl_3$. $3H_2O$. Reaction of two moles of bis[3-(indolyl)] telluride (**5**) with one mole of Na_2PdCl_4 , K_2PtCl_4 and $RhCl_3$. $3H_2O$ respectively, gave crystals of bis{bis[3-(indolyl)] telluride} palladium(II) chloride (**8**) , bis{bis[3-(indolyl)] telluride} platinum(II) chloride (**9**) and bis{bis[3-(indolyl)] telluride} rhodium(III) chloride (**10**), respectively, as yellow to yellowish brown crystals in 68-76% yields, *Scheme* 2.



***Scheme* 2:-** preparative methods of complexes **8-10**

Generally, the prepared organotellurium based on indole compounds **1-10** are colored, solids, stable in air, soluble in DMF and DMSO. The complexes **8-10** are soluble in water which can be as an evidence to the ionic nature of these complexes.

The CHN analysis of these compounds **1-10** are in good agreement with calculated values, which indicated the suggested structures are correct.

The molar conductance of all synthesized compounds **1-10** in were measured in 1×10^{-3} M of DMSO solutions at room temperature . The molar conductance of 3-(indolyl) mercuric chloride (**1**), 3-(Indolyl) tellurium tribromide (**2**), bis[3-(Indolyl)]tellurium dibromide (**3**), bis[3-(indolyl)tellurium dichloride (**6**) and bis[3-(indolyl)tellurium iodide (**7**) were found at 33.20, 27.60 , 23.40 , 21.00 and 34.00 ohm^{-1} cm^2 mol^{-1} respectively. This indicate that these compounds behave as 1:1 electrolyte which are in agree well with previous works in DMSO solution. [15-18] These observations may be due to ionic character of Hg-Cl and one of the Te-halide bonds in these compounds. The molar conductance of bis [3-(indolyl)] ditelluride (**4**) and bis [3-(indolyl)] telluride (**5**) were found at 3.00 and 4.70 ohm^{-1} cm^2 mol^{-1} respectively. These values confirm that these compounds are nonelectrolytes. [12- 14] On the other hand, the molar conductance of complexes (**8-10**) were found 51.00, 58.00 and 79.00 ohm^{-1} cm^2 mol^{-1} respectively. These data indicate that complexes (**8**) and (**9**) behave as 1:2 electrolytes while complex (**10**) behave as a 1:3 electrolyte which are agreed well with the suggested structures of complexes. [12-14]

The IR spectra of all prepared compounds (**1-10**) display common feature in certain region and characteristic bands in the fingerprint and other regions. The IR spectral analysis of compounds (**1-10**) is in good arrangement with the suggested structures. The IR spectra of compounds **(2-7)** are quite similar to those of 3-(indolyl) mercuric chloride **(1**) which indicated that telluration has been occurred at the mercuration position. The IR spectra of all prepared compounds **(1-10)** shows stretching vibration of υ(N-H) for pyrrole moiety as a broad and strong band in the range 3386-3481 cm^{-1} which indicates that there is no substitution occurred on the nitrogen of pyrrole ring, and it is broad band due to strongly hydrogen bonding in the solid state while the high intensity of this band reflects the donation of electrons from the nitrogen atom to the indole nucleus. [15] This band together with the band in the range 1512 - 1558 cm^{-1} can be ascribed to be the stretching and deformation vibrations of the N-H bond. [16] These results imply that there were still N-H bonds on the backbone of the entire prepared compounds. Thus, nitrogen species could not be the substitution site, and substitution should happened at the 2 and 3-positions. The C=C (in ring) aromatic asymmetrical stretching vibration peaks were observed in the range 1694- 1643 cm^{-1} region whereas the C=C symmetrical stretching peaks were observed in the range 1558- 1512 , these values are in good agreement with previous works. [17, 18] The peak at the range 3064 -3132 cm-1 can be attributed to stretching vibration of aromatic C-H bond. The band at 742-750 cm-1 indicates that the benzene ring is not affected during the reaction process of indole. [16] The FT-IR region below 1000 cm^{-1} at 609 cm^{-1}, 731 cm^{-1} and 744 cm^{-1} exhibits the out of plane bending of C-H bond vibrations of aromatic carbon double bonds(=C-H). The band at 742- 750 cm^{-1}indicates that the benzene ring is not affected during the reaction process of indole. The IR spectra of compounds **(1-10**) show week bands in the range 455-588 cm-1 due to υ(Te-C) vibration. [11] Comparison IR spectra of complexes **8**, **9** and **10** with compound **5**, a high frequency shift (9-37cm^{-1}) was appeared can be attributed to coordinate of nitrogen atoms of compound **5** with palladium, platinum and rhodium ions respectively. Also, IR spectra of complexes **8**, **9** and **10** show a weak band at 460, 435and 455 cm^{-1} respectively with low frequency which indicate to coordinate tellurium atom of compound 5 with palladium, platinum and rhodium ions respectively. The IR spectra of compound **5** show a weak band at 457 cm-1assign to ν(C-Te). The same band was shifted toward low frequency (9-22 cm^{-1}) in complexes **8-10** which can be as evidence to coordinate compound **5** with palladium, platinum and rhodium ions respectively. [19, 20]

^1H NMR spectra of compounds **1-10** were recorded in DMSO-d_6. ^1H NMR spectra of indoles have been thoroughly investigated, and interpreted in considerable detail. Since the indole nucleus bears relatively few hydrogens, and their environment changes significantly according to the position on the nucleus, it is frequently possible to assign every proton in the spectrum of a simple indole and to determine the positions of substitution on the nucleus. Generally, the chemical shifts of pyrrole ring protons are less than that in the benzene ring(except proton of nitrogen atom). Also, the 2 and 3 protons are less deshielded and appear at higher fields than the other protons, with the considerable electron density at 3 being reflected in the higher field of this proton, despite the fact that it is deshielded more by the benzene ring current than is the 2 proton. Protons at 5 and **6** appear next in order, followed by those at 7 and 4 which are strongly deshielded by the currents in both rings. The ^1H NMR spectra of compounds **1-10**show a doublet signal centered at the range 8.36- 8.87 ppm due to N-H. Based on these observation, the chemical shift of N-H proton of free indole (10.10ppm), [21] are shifted toward high field compared with the N-H proton of indole moiety of the unsymmetrical telluride compounds. This may be due to the attachment of this ring with another aromatic rings. The appearance of N-H resonance signal in all the prepared compounds **1-29**, it means that the N-H bond has no substitution which in well accordance with the FT-IR results . ^{1}H NMR spectra of compounds **1-10** further proved that the substitution of indole ring at 3-position by disappearance the resonance signal of H_3 at 6.1 ppm. This can be as an evidence that mercuration substitution located upon C-3. ^{1}H NMR spectra of compounds **1-10** show a multiple signals pointed at the range 6.733-8.306ppm can be assigned to H_2. The multiplets of the H_2 signal are particularly simplified, demonstrating that the NH proton is strongly coupled to this proton. ^{1}H NMR spectra of compounds **1-10** show two closed signals at the range 7.367-7.709 and 7.259- 7.403 ppm can be attributed to H_5 and H_6, respectively. ^{1}H NMR spectra of compounds **1-10** show two doublet signals at the range 7.874- 8.370 and 7.605-8.150 ppm can be assigned to H_4 and H_7, respectively.

The mass spectra of all organotellurium compounds based on indole **1-10** were recorded at 70 eV and provided further support for their suggested structures. The first electron removed from the prepared compounds **1-10** under electron impact probable originates from the nitrogen atom to form ionic peak at $[M-1]^+$ 351, 482, 518, 242, 358, 429, 612, 896, 984and 928, respectively. The ionic peaks confirm the suggested structures for the prepared compounds **1-10**. The mass spectra of compound **4** show a high intensity peak at m/e 242 due to the ion $[C_8H_5NTe]^+$ cleavage of Te-Te bond. The mass spectra of compounds **3** and **5-10** show low intensity peak due to [M-2] at m/z at, 517, 357, 428, 611, 895, 983 and 927, respectively. The mass spectra of all prepared compounds **1-10** show low intensity peak at 350, 481, 515, 241, 355, 426, 609, 889, 977 and 921 respectively can be attributed to lose of proton in position 2 in pyrrole ring. The mass spectrum of compound **1** show a peak at m/z 115 can attributed to the $[C_8H_5N]$ ion due to lose of HgCl group. The mass spectra of compounds **2**, **3**, **6**, **7** shows a peak at 401, 435, 391, 482 due to lose one halogen atom. This observations can be explained to the fact that there is difference in the bond strength of halogens bonds which binding with tellurium atom in organotellurium compounds. The same spectra of compounds **2**, **3**, **6** and **7** were showed a peak at 241, 355, 355, 355 attributed to subtract the other halogen atoms (Br_2, Br, Cl and I respectively). Also, the mass spectra of compounds **8**, **9** and **10** exhibit a peak at 106, 195 and 102 can be attributed to metal Pd, Pt and Rh, respectively. The mass spectra of compounds **1-10** show peaks at m/z 78, 66 and 52 can be assigned to ions $[C_6H_5]^+$, $[C_5H_5]^+$ and $[C_4H_4]^+$, respectively.

The UV-Vis spectra of compounds **1-10** were measured at 1 x 10^{-4} M using dimethyl formamid (DMF) as a solvent. The U.V. Visible absorption spectra of indole derivatives are highly characteristic and sensitive to changes in substitution on the indole nucleus they are therefore important in the identification of indole structures ,and have been a particularly valuable aid in the classification of indole derivatives. The U.V-Visible spectra of compounds **1-10** show three main absorption peaks in the regions(278-265 nm), (308- 292 nm) and (317- 310 nm) due to $\pi \rightarrow \pi^*$ transition bands. For complexes **8-10**, all the $\pi \rightarrow \pi^*$ transition bands showed a hyperchromic effect with a slight red shift compared with compound 5 (*i.e.* the ligand). These changes can be considered as an evidence for the coordination of compound 5 to Pd(II), Pt(II) and Rh(III) metal ions respectively. In the spectra of complexes **8-10**, there also appeared a new band in the visible region in the range (482-429 nm) can be assigned to charge transfer.

Table 1:- Elemental analysis CHN and ^{1}H NMR data for some new organotellurium compounds based on indole.

Comp. No.	Elemental analysis %Found (calcd.)			^{1}H NMR (DMSO-d_6); TMS = 0ppm
	C	H	N	
1	27.24 (27.28)	1.74 (1.72)	4.03 (3.98)	8.418(d, NH, 1H , *J*= 8.0 Hz), 8.270 (t, H_4,1H , *J*= 9.2 Hz), 7.944 (d, H_7, 1H , *J*=3.6 Hz) 7.701(d, H_5, 1H , *J*=7.6 Hz), 7.400 (d, H_6, 1H , *J*=7.2 Hz), 7.347(d, H_2, 1H, *J*=8.0 Hz)
2	19.82 (19.87)	1.27 (1.25)	2.93 (2.90)	8.421(d, NH, 1H , *J*= 8.0 Hz), 8.271 (t, H_4,1H , *J*= 9.2 Hz), 7.945 (d, H_7, 1H , *J*=3.6 Hz) 7.709(d, H_5, 1H , *J*=7.6 Hz), 7.403 (d, H_6, 1H , *J*=7.2 Hz), 7.340(d, H_2, 1H, *J*=8.0 Hz)
3	37.02 (36.98)	2.35 (2.33)	5.36 (5.39)	8.381(d, NH & NH', 2H , *J*=7.6 Hz), 7.874(d, H_4&H_4', 2H , *J*=7.6 Hz), 7.710(s,H_7&H_7', 2H) 7.367(d, H_5& H_5', 2H, *J*=8.8 Hz), 7.331(d, H_6& H_6', 2H, *J*=4.4Hz),

				7.297(d, H_2& H_2' , 2H, *J*=7.2 Hz)
4	39.40 (39.42)	2.51 (2.48)	5.80 (5.75)	8.826(d, NH &NH', 2H , *J*=8.4 Hz), 8.370(d, H_4&H_4', 2H , *J*=8.4 Hz), 7.705(s,H_7 & H_7', 2H , *J*=8.0 Hz) 7.375(d, H_5 & H_5' , 2H, *J*=10.8 Hz), 7.293(d, H_6 & H_6' , 2H, *J*=7.6 Hz), 7.204(d, H_2 & H_2', 2H, *J*=6.8 Hz)
5	53.37 (53.40)	341 (3.36)	7.81 (7.78)	8.85(d, NH & NH', 2H , *J*=8.0 Hz), 8.050(t, H_4 & H_4', 2H , *J*=8.0 Hz), 7.605(d, H_7&H_7', 2H , *J*=12 Hz) 7.435(d, H_5& H_5' , 2H, *J*=12.0 Hz), 7.260(d, H_6 & H_6' , 2H, *J*=8.0 Hz), 6.750-6.690(m, H_2 & H_2', 2H)
6	44.59 (44.61)	2.77 (2.81)	6.48 (6.50)	8.419(d, NH, 1H , *J*= 8.0 Hz), 8.260 (t, H_4,1H , *J*= 9.2 Hz), 7.913 (d, H_7, 1H , *J*=3.6 Hz) 7.701(d, H_5, 1H , *J*=7.6 Hz), 7.400 (d, H_6, 1H , *J*=7.2 Hz), 7.335(d, H_2, 1H, *J*=8.0 Hz)
7	31.28 (31.31)	2.01 (1.97)	4.54 (4.56)	8.417(d, NH, 1H , *J*= 8.0 Hz), 8.200 (t, H_4,1H , *J*= 9.2 Hz), 7.934 (d, H_7, 1H , *J*=3.6 Hz) 7.701(d, H_5, 1H , *J*=7.6 Hz), 7.400 (d, H_6, 1H , *J*=7.2 Hz), 7.330(d, H_2, 1H, *J*=8.0 Hz)
8	42.68 (42.84)	2.67 (2.70)	6.24 (6.25)	8.351(d, 2NH &2NH', 4H , *J*=8.0 Hz), 8.150(d, $2H_4$& $2H_4$', 4H , *J*=7.2 Hz), 7.571(d,2 H_7&$2H_7$', 4H , *J*=7.6 Hz) 7.315-7.259 (m, H_5 , H_6, H_5'&H_6' ,4H), 6.733(d, $2H_2$ & $2H_2$', 4H, *J*=8.4 Hz)
9	39.02 (38.99)	2.42 (2.45)	5.65 (5.68)	8.443(d, 2NH & 2NH', 4H , *J*=8.4 Hz), 8.255(s, $2H_4$ & $2H_4$', 4H), 7.917(d, $2H_7$ & $2H_7$', 4H , *J*=4.0 Hz) 7.484 (d, $2H_5$ &$2H_5$' ,4H, *J*=2.2 Hz), 7.309(d, $2H_6$ & $2H_6$' , 4H, *J*=9.2 Hz), 8.306(d, $2H_2$ & $2H_2$', 4H, *J*=4.0 Hz)
10	41.40 (41.37)	2.57 (2.60)	6.08 (6.03)	8.349(d, 2NH &2NH', 4H , *J*=8.0 Hz), 8.144(d, $2H_4$& $2H_4$', 4H , *J*=7.2 Hz), 7.562(d,2 H_7&$2H_7$', 4H , *J*=7.6 Hz) 7.314-7.248 (m, H_5 , H_6, H_5'&H_6' ,4H), 6.726(d, $2H_2$ & $2H_2$', 4H, *J*=8.4 Hz)

Optimized Structures:-

The optimized B3LYP/6-31G* structures for all the prepared compounds (**1-10**) are presented in *Figure* 1. In the figures, the grey spheres are C atoms, the white spheres are H atoms, blue spheres are N atoms, red spheres are Br atoms, green sphere are chloride atoms and orange spheres are Te atoms.

In compound **1** the molecule geometry is planner where the chlorine and mercury and indolyl group lie in the same plane (*i.e.* the bond angle 180 ^{0} , the halogen atoms (Cl, Br and I) lie on the Z-axis with central atom(tellurium atom)). The molecular geometry of compound **2** bipyramid arrangement (seesaw molecular geometry) where the tellurium atom and the bromide atoms lie in the same triangle plane while the indolyl goup and lone pair lay perpendicular around the triangle plane (*i.e.* inolyl , tellurium and bromine atoms in bond angle 90 ^{0}). The molecular geometry of compound 3, the bond angle between two indolyl groups and tellurium atom is 111 ^{0} C, while between lone pair , tellurium atom, and indolyl group is 139 ^{0}). The bond angle between two bromine atoms and tellurium atom is 180 ^{0}, so, the molecular geometry of compound 3 must be in bipyramidal arrangement(seesaw molecular geometry). The molecular geometry of dichloride (*i.e.* **6**) and diiodide(*i.e.* **7**) are in agree well with compound **3**. For the ditelluride molecule(*i.e.* compound **4**) the indolyl groups in opposite sides and they lie in two different planes. The bond angles between indolyl group and two tellurium atoms are same about 101.5^0. The complexes **8**, **9** and **10** have two groups of indolyl centered in the xy plane. The molecular geometry of complexes **8**, **9** and **10** are supposed to be octahedral where the bis[3-(indolyl)]telluride ligand **(i.e. compound 5)** behave as a tridentate ligand. Some of the selected structural parameters (charges and bond lengths) of the optimized geometries are listed in Table 2.

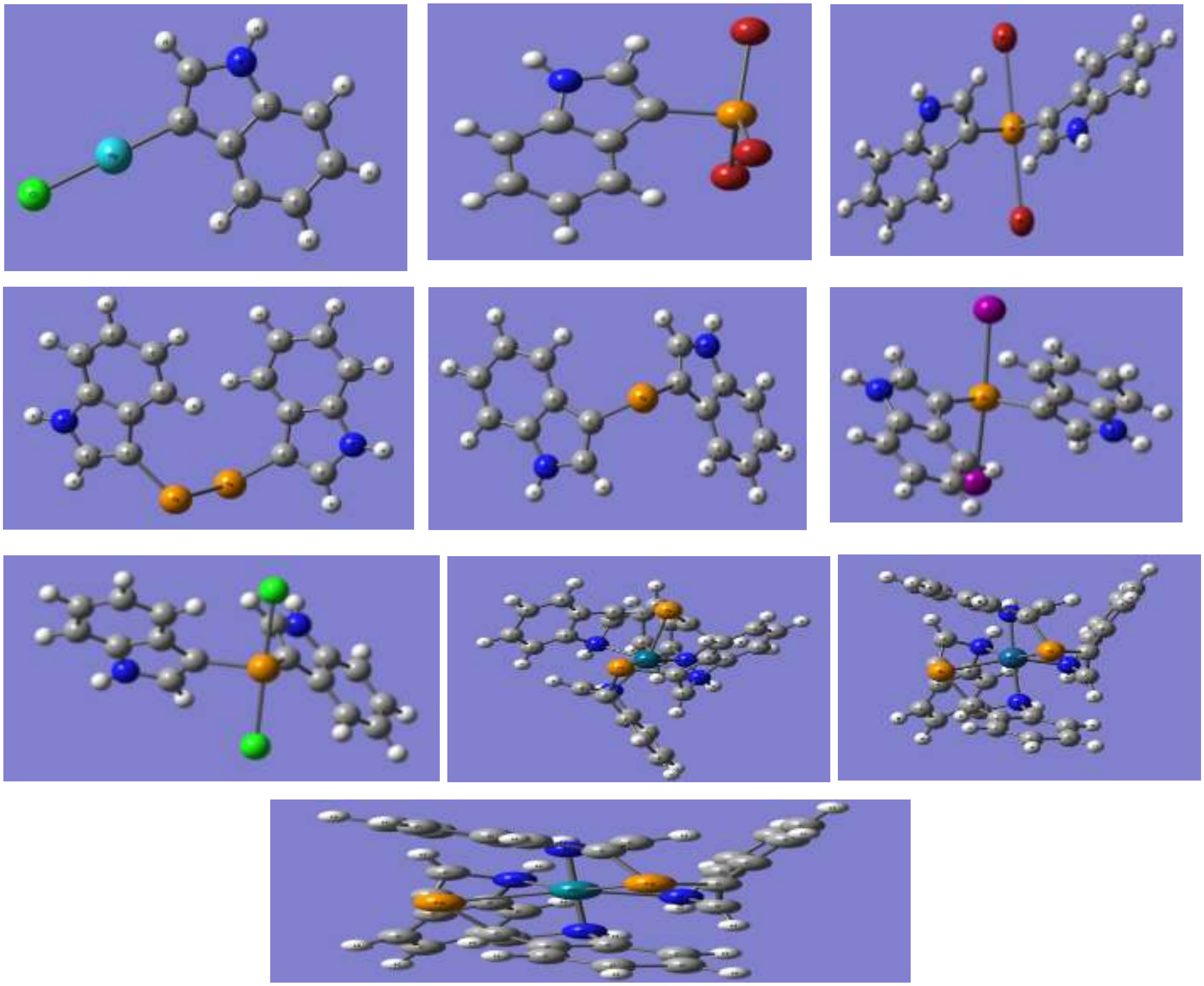


Figure 1:- The structures of compounds **1**- **10** optimization have been performed by B3LYP/3-21G* method.

Electrostatic Potential Isosurface:-

The three-dimensional mapped isosurface of the electrostatic potential for selected compounds **2** and **5** is shown in *Figure* 2. This plot provides information on the reactivity of the molecules in actual reactions with electrophiles or nucleophiles. Dark (shadow) colors indicate positive ESP regions and light (yellow) colors indicate negative ESP regions.

In general, for the isomers calculated, the plots show that the tellurium atom has a positive and negative ESP region. This suggests that the tellurium atom can be more easily oxidized and reduced between valence state II and IV. The Br atom has a more negative ESP region, while the N and phenyl rings have less negative ESP regions. This is very important to understand of the physical properties for the molecules studied.

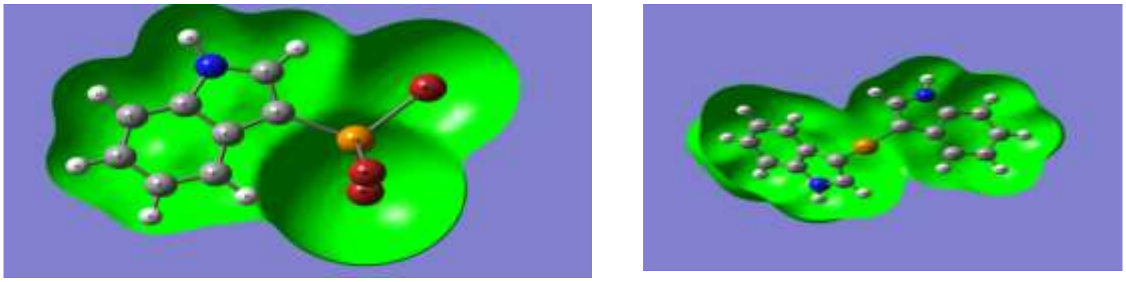


Figure 2:- Three dimensions isosurface plots of the electrostatic potential for compounds **2** and **5**.

Table 2:- Selected structural parameters (charges, bond lengths and angles) of the prepared compounds **1-10**.

Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Charge										
7C	-0.293	-0.464	-0.435	-0.420	-0.386	-0.352	-0.314	-0.471	-0.446	-0.436
8C	-0.172	-0.172	-0.164	-0.224	-0.245	-0.290	-0.282	-0.137	-0.151	-0.157
15N	-0.639	-0.398	-0.410	-0.392	-0.395	-0.380	-0.379	-0.504	-0.562	-0.525
					Bond length					
1C-7C	1.45777	1.45950	1.45592	1.45508	1.45517	1.45558	1.45518	1.46462	1.47598	1.47598
7C-8C	1.36938	1.40209	1.39011	1.36804	1.36556	1.36991	1.37119	1.26928	1.27489	1.27489
8C-15N	1.38444	1.37190	1.38291	1.37949	1.38270	1.36609	1.36506	1.42543	1.42498	1.42498
2C-15N	1.38603	1.40714	1.40203	1.38965	1.38799	1.39196	1.39243	1.53426	1.52676	1.52676
7C-M	2.08678	2.06944	2.09136	2.08805	2.09738	2.06979	2.07039	1.96650	1.97969	1.97969
Te-M								1.96650	2.77604	2.77604
N-M								2.13486	2.13335	2.13335
Totel energy	-416.914	-410.7	-764.2	-742.4	-734.3	-764.1	-757.05	-1593.9	-1586.3	-1576.7
Dipole moments	5.8298	7.0124	6.3540	0.8317	2.4975	8.1183	8.3281	4.0505	3.8187	4.7441

Experimetal:-

Synthesis:-

***Synthesis of 3-(indolyl) mercuric chloride* (1):**

3-(Indolyl) mercuric chloride was synthesized according to the literature with some modifications. [8]

Mercuric acetate (6.80g, 21.00 mmol) in 30 mL of ethanol was added dropwise to a solution of indole(2.50g,21.00mmol) in the same solvent 30 mL. The mixture was refluxed for 1 h. The hot mixture was filtered. The filtrate was treated with saturated sodium chloride (5.2 g, 86 mmol) with stirring for 30 min. A white precipitate was obtained and collected by filtration. The crude solid was washed several times with methanol and dried under vacuum. White crystals of 3-(indolyl) mercuric chloride (1) in 77% yield , M.p.183-185 ^{0}C(lit. ^{0}C).

IR(KBr) cm^{-1}: 3330 br, 3132 w, 1649 s, 1521 m, 1228 s, 675 s, 638 m, 594 m. UV-Vis[λmax, nm(ε M^{-1}. cm^{-1})]: 272(12070), 292(12337), 310(14650) . Molar conductivity Λ_m Ohm^{-1}. Cm^2.Mol^{-1} : 33.20 . R_f (TLC): 0.79 . Mass spectra M/ z (70 ev): 351.18, 315.72, 116.06, 78.05, 69.06, 66.10, 52.07.

Synthesis of 3-(indolyl)tellurium tribromide (**2**):-

A solution of 3-(indolyl)mercuric chloride(1) (1.57 g,4.47 mmol) in 20 mL sodium dried dioxane was added drop by drop to a solution of tellurium tetrabromide (2.00 g, 4.47 mmol) in 30 mL of the same solvent was refluxed for 6 h under argon atmosphere. On cooling a 2:1 complex of dioxane and mercury (II) halide was separated as white plates and removed by filtration. The filtrate was evaporated by a rotary evaporator to give a bright brown precipitate. Recrystallization of the crude product using a mixture of chloroform and methanol (7:3) gave a light brown solid of 3-Indolyltellurium tribromide (2) in 69% yield. M.p.185-187^0C. IR(KBr) cm^{-1}: 3386 br, 3122 w, 3025 w, 1689 s, 1519 m, 1222 s, 675 m, 588 w. UV-Vis[λmax, nm(ε M^{-1}. cm^{-1})]: 270 (16250), 300(14930) , 3159 (14000) . Molar conductivity Λ_m Ohm^{-1}. Cm^2.Mol^{-1} : 27.60. R_f (TLC): 0.81 . Mass spectra m/ z (70 ev): 482.71, 403.80 , 321.87, 357.82 , 276.87 , 198.96 , 116.06, 78.05, 69.06, 52.07.

Synthesis of bis[3-(indolyl)]tellurium dibromide **(3):-**

3-(indolyl) mercuric chloride (1) (0.78 g,2.23 mmol) and tellurium tetrabromide (2.00 g, 4.47 mmol) were refluxed in dry dioxane (30 mL) for 6h under argon atmosphere. The reaction mixture was filtered hot. The filtrate deposited a 2:1 complex of HgClBr $(dioxane)_2$ as a white plates upon cooling to room temperature. The white complex was filtered off. The filtrate was poured into 500 mL of ice - water to obtain a brown precipitate immediately. The resulting precipitate was collected by filtration and twice recrystallized from a mixture of methanol and chloroform (4:1) to afford yellowish brown crystals in 71% Yield, M.p. 127-129^0C. IR(KBr) cm^{-1}: 3431 br, 3118 w, 1685 s, 1542m, 1288 m, 669m, 580 w. UV-Vis[λmax, nm(ε M^{-1}. cm^{-1})]: 272(16739), 308(80830), 315(59770). Molar conductivity Λ_m Ohm^{-1}. Cm^2.Mol^{-1} : 23.40. R_f (TLC): 0.80. Mass spectra m/ z (70 ev): 518.84, 435.93, 355.01, 314.01, 283.98, 246.96, 232.10, 202.08, 148.10, 116.06 78.11, 66.10, 52.07.

Synthesis of bis[3-(indolyl)] ditelluride (4):-

(3-Indolyl) tellurium tribromide (2) (1.00g, 2.06 mmol) was refluxed in 25 mL of ethanol. An ethanolic solution of hydrazine hydrate was added dropwise to the refluxing solution until the evolution of nitrogen was ceased. The resulting solution was cooled to room temperature and poured into 100 mL of distilled water and extract with diethyl ether (4 × 30 mL). The etheric extracts were dried over an anhydrous calcium chloride. Evaporation of solvent afforded a dark red solid. The crude product was recrystallized from a mixture of methanol and dichloromethane (1:4) to obtain dark red crystals in 55%, M.p. 148-150^0C. IR (KBr) cm^{-1}:3448 br, 3182 w, 1650 s, 1558 m, 1215 s, 671 m, 466 w. UV-Vis [λmax, nm (ε M^{-1}. cm^{-1})]: 274(14600), 300(13097), 314 (13008). Molar conductivity Λ_m Ohm^{-1}. Cm^2.Mol^{-1} : 21.00 . R_f (TLC): 0.80 . Mass spectra m/ z (70 ev): 491.91, 362.85, 362.01, 281.04, 232.10, 202.08, 196.95, 130.08, 116.09, 97.09, 81.06, 78.11, 78.08, 52.06.

Synthesis of bis[3-(indolyl)]telluride **(5):-**

Bis[3-(Indolyl) tellurim dibromide (3) (1.00g, 1.92 mmol) was dissolved in 20 mL of ethanol and refluxed. A solution of hydrazine hydrate in ethanol was added dropwise to the refluxing solution until the evolution of nitrogen was ceased. The resulting solution was poured into 500 mL of distilled ice - water to afford a green solid. The crude product was twice recrystallized from a mixture of methanol and chloroform (1:3) to obtain a dark green solid in 59 % yield, M.p.118-120 ^{0}C. IR (KBr) cm^{-1}:3444 br, 3112 w, 1649 m, 1558 m, 1215 s, 703 m, 622 m, 586 m, 457 w. UV-Vis[λmax, nm(ε M^{-1}. cm^{-1})]: 265(17847), 295(9858), 310(7140) . Molar conductivity Λ_m Ohm^{-1}. Cm^2.Mol^{-1} : 34.00 . R_f (TLC): 0.92 . Mass spectra m/ z (70 ev): 362.01, 359.99, 316.02, 202.08, 178.08, 149.12, 116.06, 79.06, 78.11, 66.10, 52.07.

Synthesis of bis[3- (indolyl)]tellurium dichloride **(6):-**

Thionyl chloride (0.12 g ,1.00 mmol) in 15 mL of dry ether was added drop by drop to an etheric solution of bis[3-(indolyl)]telluride (5)(0.39g ,1.008 mmol) with stirring at room temperature for 30 minutes. A yellow precipitate was formed immediately. Recrystallization from a mixture of methanol and chloroform (1:4) gave an yellowish brown solid of compound (**6**) in 82% Yield, M.p. 148-150 ^{0}C. IR (KBr) cm^{-1}: 3446 br, 3112 w, 1643 s, 1512 m, 1224 s, 578 m, 455 w . UV-Vis [λmax, nm(ε M^{-1}. cm^{-1})]: 272(19098), 299(16734), 310(13254) . Molar conductivity Λ_m Ohm^{-1}. Cm^2.Mol^{-1} : 3.00 . R_f (TLC): 0.86**.** Mass spectra m/ z (70 ev): 429.78, 391.32, 355.01, 314.01, 283.98, 246.96, 232.10, 202.08, 148.10,

116.06, 78.11, 66.10, 52.07.

***Synthesis of bis[3-(indolyl)]telluruim diiodide* (7):-**
A solution of iodine (0.114 g,0.45mmol) in diethyl ether 10 ml was added to a solution of bis [3-(indolyl)]telluride (5) (0.16 g, 0.45 mmol) in diethyl ether 25ml with stirring at room temperature for 30 min. gave brown solid immediately. The crude product was recrystallized by a mixture of methanol and chloroform (3:1) to afford brown crystals of compound (7) in 85%. M.p .138-140 ^{0}C. IR (KBr) cm^{-1}: 3421 br, 3118 w, 1649 s, 1554 m, 1261 s, 640 m, 617 m, 586 m, 457 w.

UV-Vis [λmax, nm(ε M^{-1}. cm^{-1})]: 274(14900), 308(14306), 312 (12700). Molar conductivity Ohm^{-1}. Cm^{2}.Mol^{-1} : 4.70 . R$_f$ (TLC): 0.84**.** Mass spectra m/ z (70 ev): 613.69, 484.77, 355.01, 314.01, 283.98, 246.96, 232.10, 202.08, 148.10, 116.06, 78.11, 66.10,.

***Synthesis of bis{bis[3-(indolyl)]telluride}palladium(II) dichlorid* (8):-**
To a stirring solution of sodium tetrachloropalladinate(II), Na_2PdCl_4, (0.50g,1.70mmol) in distilled water (30mL) a solution of bis[3-indole]telluride (5) (1.20g, 3.40 mmol) in 25mL of ethanol. The mixture was stirred at room temperature for 6h under nitrogen atmosphere to give a brown solid which was collected by filtration. The crude solid was recrystallized (twice) from a methanol to afford yellowish brown crystals in 70 % yield, M.p. >300 ^{o}C (dec.). IR (KBr) cm^{-1}: 3418 br, 3064 w, 1649 s, 1517 m, 1207 s, 634 m, 524 w. Uv-Vis [λmax, nm(ε M^{-1}. cm^{-1})]: 276(13345), 305(11025), 317(10059), 429(3316). Molar conductivity Λ_m Ohm^{-1}. Cm^{2}.Mol^{-1} : 51.00 . R$_f$ (TLC): 0.76. Mass spectra m/ z (70 ev): 896.05, 889.05, 854.05, 818.05, 357.01, 232.10, 202.08, 166.08, 148.10, 116.06, 78.11, 66.10, 52.07.

***Synthesis of bis{bis[3-(indolyl)]telluride}platinum(II) dichloride* (9):-**
This complex was prepared by the same above method of complex (8) by reacting bis[3-Indole]telluride (0.85 g, 2.40 mmol) and potassium tetrachloroplatinate(II), K_2PtCl_4, (0.5g, 1.20 mmol). Yellow crystals were obtained of compound (9) in 76% yield (0.50g, 0.67mmol), M.p. 240-242^{0}C (dec.). IR (KBr) cm^{-1}: 3420 br, 3078 w, 1694 s, 1552 m, 1267 s, 675 m, 638 m, 594 m, 511 w. UV-Vis [λmax, nm(ε M^{-1}. cm^{-1})]: 276(8219), 303(6351), 317(5748) , 430(2016). Molar conductivity Λ_m Ohm^{-1}. Cm^{2}.Mol^{-1} : 58.00 . R$_f$ (TLC): 0.83. Mass spectra m/ z (70 ev): 984.92, 976.92, 942.91, 906.95, 554.96, 357.01, 232.10, 202.08, 166.08, 148.10, 116.06, 78.11, 66.10, 52.07.

***Synthesis of bis{bis[3-(Indolyl)]telluride}rhodium(III) trichloride* (10):-**
This complex was prepared by the same above method of complex (8) by reacting bis[3-Indole]telluride (0.27 g,0.76 mmol) and rhodium(III) chloride trihydrate, $RhCl_3.3H_2O$, (0.10g, 0.38mmol). Yellowish brown crystals were obtained of compound (**10**) in 68% yield, M.p. 162-164 ^{0}C. IR (KBr) cm^{-1}:3419 br, 3078 w, 1693 s, 1552 m, 1261 s, 675 m, 588 m, 455 w. UV-Vis [λmax, nm(ε M^{-1}. cm^{-1})]: 278(19888), 303(15336), 316(11804), 482(3500). Molar conductivity Λ_m Ohm^{-1}. Cm^{2}.Mol^{-1} : 79.00. R$_f$ (TLC): 0.83. Mass spectra m/ z (70 ev): 926.78, 892.82, 857.86, 822.89, 462.90, 357.01, 314.01, 232.10, 202.08, 184.10, 166.08, 116.06, 78.11, 66.10, 52.07.

Physical Measurements:-
Analysis for C, H, and N was done by the Analytical Service Unit at Al-al-Bayt University, Jordan. FT-IR spectra were recorded as KBr disks using a FT-IR spectrophotometer Shimadzu (Japan) model 8400S in range 4000-400 cm^{-1} at General Company for Petrochemical Industries of Basrah. ^{1}H NMR spectra were recorded at University of Isfahan Isfahan, Islamic Republic of Iran by using a Bruker 400 MHz (Germany). Chemical shifts of all ^{1}H NMR spectra were recorded in δ (ppm) unit downfield from the internal reference tetramethylsilane (TMS), using DMSO-d_6 solvents, J values are given in Hz. Mass spectra were recorded at University of Isfahan, Isfahan, Islamic Republic of Iran, by using a MS model 5975C VL MSD. UV-Vis spectrum were recorded at Department of Chemistry, College of Science, University of Basrah by using Scan 80D (England) at range 200-800 nm using *N,N*-dimethylformamide as a solvents and 1 cm^{3} pathway quartz cells. The molar conductivity for some synthesized compounds were measured in 1×10^{-3}-1×10^{-5} M solutions of dimethylsulfoxide solvent at room temperature using a Konduktoskop model 365B using standard conductivity cell with constant equal to 0.81 cm^{-1}. Melting points were determined on a Gallenkamp melting point apparatus and are uncorrected.

The calculations presented in this work were carried out by using the GAUSSIAN03 suite of programs . [22] The hybrid Becke 3-Lee–Yang–Parr (B3LYP) exchange correlation functional was applied for DFT calculations . [23-25] The geometries of the compounds and the frequencies were evaluated with the B3LYP/3-21G* theory method.

Conclusions:-

In summary, we have prepared six compounds for organotellurium based on indole by transmetallation reaction of 3-(indolyl) mercuric chloride with tellurium tetrabromide in 1:1 and 1:2 mole ratio in dry dioxane gave the corresponding tribromide and dibromide, respectively, in good yields. Reaction of compounds tribromide and dibromide can be converted to the corresponding ditelluride and telluride, respectively, by action of ethanolic hydrazine hydrate. Furthermore, the ligand properties of bis[8-(quinolyl)] telluride with with Pt(II), Pd(II) and (III) ions gave NTeN coordination type with octahedral geometry.

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