Synthesis, Characterization and Theoretical Investigation of Innovative Charge-transfer Complexes Derived from the N-phenyl 3,4-selenadiazo Benzophenone Imine

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Abstract:

In the current study, a direct method was used to create a new series of charge-transfer complexes of chemicals. In a good yield, new charge-transfer complexes were produced when different quinones reacted with acetonitrile as solvent in a 1:1 mole ratio with N-phenyl-3,4-selenadiazo benzophenone imine. By using analysis techniques like UV, IR, and ^{1}H, ^{13}C-NMR, every substance was recognized. The analysis's results matched the chemical structures proposed for the synthesized substances. Functional theory of density (DFT) has been used to analyze the molecular structure of the produced Charge-Transfer Complexes, and the energy gap, HOMO surfaces, and LUMO surfaces have all been created throughout the geometry optimization process utilizing the base set of 3–21G geometrical structures. The molecular geometry and contours for compounds with charge-transfer complexes have been evaluated during the process of geometrical optimization. By investigating the interactions between donor and acceptor, we have also been contrasting the energies (HOMO energies) of the chemicals in charge-transfer complexes. For molecules containing charge-transfer complexes, the lower case, electronegativity, ionization potential, electron affinity, and electrophilicity have all been calculated and studied.

Keywords: Charge-transfer Complexes, Different quinones, Energy gap, HOMO energies, N-phenyl 3,4-selenadiazo benzophenone imine.

Introduction:

Organic complexes of charge-transfer consist of two systems formed by a pair of electrons with a specified stoichiometry- an electron donor and an electron acceptor unit. For many years, charge-transfer complexes have been thoroughly studied in an attempt to develop standards for creating materials with high room-temperature mobility or superconductivity [1]. However, in recent years, attention has also been given to the creation of more technologically advanced applications utilizing such charge-transfer complexes [2-4]. As an example, ferroelectrics [5], photoconductors [6,7], light detectors [8], strain sensors [9], thermoelectric [10], transistors of organic field-effect (OFETs), where CT complexes can function as organic metals [11,12] or organic semiconductors [13,14]. Organoselenium compounds have long been demonstrated to be particularly significant chemicals from a practical standpoint, in addition to being useful intermediate products in organic synthesis and realistic models for exploring fundamental difficulties of theoretical chemistry [15-18]. Organoselenium compounds' unusual properties make them ideal as synthons because selenium-containing fragments can be easily incorporated into organic compounds and selenium atoms can be eliminated through appropriate processes, such as oxidation, which results in the formation of a double bond through synelimination of selenium oxide[19]. The majority of the reactions used to synthesis organo compounds of selenadiazole are known to be based on the interaction between organo diamine and selenium dioxide [20-22]. This study's objective is to synthesize new charge-transfer complexes by reacting five types of quinones (p-benzoquinone, p-anthraquinone, Tetrachloro benzoquinone (TCBQ), 7, 7, 8, 8-Tetracyano quino dimethane, 1,4-

Dihydroxyanthraquinon). With N-phenyl 3,4-selenadiazo benzophenone imine, to create new charge-transfer complexes compound.

Material and Methods:
Materials
The chemicals used included 3,4-diamino benzophenone (Fluka), aniline (Sigma-Aldrich), ethanol absolute and acetonitrile (Fluka.), p-benzoquinone (Sigma-Aldrich), anthraquinone (Sigma-Aldrich), Tetrachloro benzoquinone (Sigma-Aldrich), 7,7,8,8-Tetracyanoquinodimethane (Fluka.), 1,4-Dihydroxyanthraquinon (Strem chemicals Inc.), selenium dioxide powder (Strem chemicals Inc.), nitric acid (HGB).
Computational Analysis Program: Gaussian 09W set of (3–21G) basis and using estimated DFT-based descriptors.
Instrumental
Shimadzu UV-visible Spectrophotometer double-beam model UV-1650 (Japan) equipped quartz (cells 1.00 cm), Electro thermal (melting point) apparatus. ^{1}H-NMR spectra were recorded on (Bruker 500 MHz spectrometers) with TMS as an inner reference utilizing soluble DMSO-d$_6$. Infrared spectra When using KBr, the range of wave numbers is 4000-400 Cm^{-1} utilizing an FT-IR spectrophotometer, Shimadzu model 8400 S.

Procedure
1. Preparation of 3,4-Selenadiazo benzophenone(I)
An amount of (20 mmol) 4.24 g of 3,4-diamino benzophenone was dissolved in (30 ml) of ethanol and mixed with (20 mmol) 2.2 g of selenium dioxide dissolved in 30 ml of ethanol. By using a round bottom flask, the mixture was refluxed in a water bath for 2 hours until a coffee-colored solution is formed. After that, the cooled solution was then filtered and washed with hot ethanol to obtain a coffee-colored precipitate with an 80% yield and an M.P (melting point) of 95°C. Rf value=0.78 (7:3) (Ethyl acetate\n-hexane). UV-visible spectra were recorded at 200-750 nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions. with ʎ max 225 nm, 273 nm, 355 nm. FT-IR with KBr disk: υ(C–H) Ar. = 3061 cm^{-1}, υ(C=O) Ar. = 1649 cm^{-1}, υ(C=N) Ar. = 1579-1600 cm^{-1}, υ(C=C) Ar.= 1490-1500 cm^{-1}, υ (C-Se-N) Ar. = 3260 cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6) δ Ar. $_{14}$C-H, $_{16}$C-H (2H, m, δ 7.52); Ar. $_{15}$C-H, $_{17}$C-H (2H, m, δ 7.74); Ar. $_{13}$C-H, (1H, t, δ 7.89); Ar. $_9$C-H, (1H, d, δ 7.90); Ar. $_8$C-H, (1H, d, δ 8.02); Ar. $_6$C-H, (1H, s, δ 8.11). ^{13}C NMR: Ar. $_6$C δ 126.7 (1C, s), Ar. $_9$C 127.2 (1C, s), Ar. $_{15}$C 127.8 (1C, s), Ar. $_8$C 127.9 (1C, s), Ar. ($_{14}$C, $_{16}$C) 128.4 (2C, s), Ar. ($_{13}$C, $_{17}$C) 129.0 (2C, s), Ar. $_7$C 129.3 (1C, s), Ar. $_{12}$C 137.2 (1C, s), Ar. ($_3$C, $_4$C) 160.4-160.6 (2C, 160.5 (s), 160.5 (s)), Ar. $_{10}$C 195.0 (1C, s). As shown in Scheme 1, Table 1,2 and 3, Figs.1, 8, 15 and 22.

3,4-diaminobenzophenone

Selenadiazo -3,4-diaminobenzophenone(I)

Scheme 1. Preparation of 3,4-Selenadiazo benzophenone(I)

2. Preparation of N-phenyl 3,4-selenadiazo Benzophenone Imine (II)
An amount of 0.279 g (3 mmol) of pure aniline was dissolved in 20 ml of ethanol and mixed with 0.860 g (3 mmol) of Selenadiazo 3,4-diaminobenzophenone (prepared in first step) dissolved in 20 ml of ethanol also. By using a round bottom flask, the mixture was refluxed in a water bath for 5 hours. After that, the solution was cooled, washed with cool ethanol, and filtered with a Buechner funnel to obtain a light coffee-colored precipitate with a yield of 74% and a melting point 105–110 C°. Rf value=0.93 (7: 3) (Ethyl acetate\n-hexane UV-visible spectra were recorded at 200-750 nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions with ʎ max

(220 nm, 233 nm, 240 nm, 243 nm, 250 nm, 270 nm, 345 nm). FT-IR with KBr disk: υ(C–H) Ar. = 3063 cm^{-1}, υ(C=N) Ar. = (1593-1637) cm^{-1}, υ(C=C) Ar. = 1448-1556 cm^{-1}, υ(C–N) Ar. = 1325 cm^{-1}, υ (C-Se-N) Ar. = 3250 cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6) δ Ar. $_{13}$C-H, $_{14}$C-H, $_{15}$C-H, $_{16}$C-H, $_{17}$C-H, $_{20}$C-H, $_{21}$C-H, $_{22}$C-H (8H, m, δ 7.5-7.7); Ar. $_{19}$C-H, $_{23}$C-H (2H, m, δ 8.2); Ar. $_9$C-H, (1H, d, δ 8.01); Ar. $_8$C-H, (1H, d, δ 8.03); Ar. $_6$C-H, (1H, s, δ 8.10); ^{13}C NMR: Ar. $_6$C δ 126.6 (1C, s), Ar. $_9$C 128.6 (1C, s), Ar. ($_{13}$C,$_{17}$C)124.1 (2C, s), Ar. $_8$C 129.1 (1C, s), Ar. ($_{14}$C, $_{16}$C) 130.1 (2C, s), Ar. $_{15}$C δ 127.8 (1C, s), Ar. $_{18}$C δ 132.1 (1C, s), Ar. ($_{19}$C, $_{23}$C) 129.2 (2C, s), Ar. ($_{20}$C,$_{22}$C)128.4 (2C, s), Ar. $_{21}$C δ 127.8 (1C, s), Ar. $_7$C 127.3 (1C, s), Ar. $_{10}$C 159.1(1C, s), Ar. ($_3$C, $_4$C) 160.5 (2C, 160.5 (s), 160.5 (s)), Ar. $_{12}$C 138.0 (1C,

s). As shown in Scheme 2, Table 1,2 and 3, Figs.2, 9, 16 and 23.
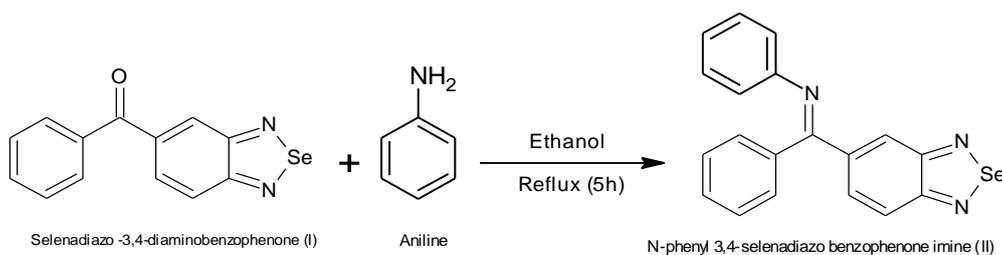
Scheme 2. Preparation of N-phenyl 3,4-selenadiazo Benzophenone Imine (II)

3. Preparing p-Benzoquino N-phenyl 3,4-selenadiazo Benzophenone Imine (III)

An amount of (2 mmol) 0.725 g of N-phenyl 3,4-selenadiazo benzophenone imine was dissolved in 30 mL of acetonitrile and mixed with (2 mmol) 0.216 g of p-benzoquinone dissolved in 30 ml of acetonitrile and heated using reflux in a water bath for 3 hours. The solution was cooled and evaporated by a rotary evaporator and washed with small amounts of acetonitrile to obtain a pure and shiny brown crystal precipitate with an 76% yield and an M.P (melting point) of 107°C. Rf value=0.92 (7:3) (Ethyl acetate\n-hexane). UV-visible spectra were recorded at (200-750) nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions with Λ max 205 nm, 230 nm, 236 nm, 270 nm, 280 nm, 355 nm. FT-IR with KBr disk: υ(C–H) Ar. =3063 cm^{-1}, υ(C=O) Ar. = 1724-1788 cm^{-1}, υ (C=N) Ar. = 1597-1639 cm^{-1}, υ (C=C) Ar. = 1504-1575 cm^{-1}, υ(C–N) Ar. =1325 cm^{-1}, υ(C-Se-N) Ar. = 3259 cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6) δ Ar. $_{13}$C-H, $_{14}$C-H (2H, m, δ 7.53), δ Ar. $_{15}$C-H, $_{16}$C-H (2H, m, δ 7.58), δ Ar. $_{17}$C-H, $_{19}$C-H, $_{20}$C-H, $_{21}$C-H, $_{22}$C-H, (5H, m, δ 7.53 -7.77), δ Ar. $_{25}$C-H,$_{26}$C-H, $_{28}$C-H, $_{29}$C-H (4H, m, δ 7.85 -7.90) Ar. $_{23}$C-H (1H, d, δ 7.52); Ar. $_9$C-H, (1H, d, δ 8.01);Ar. $_8$C-H, (1H, d, δ 8.02); Ar. $_6$C-H, (1H, s, δ 8.10); as show in Scheme3, Tables.1,2 and 3, Figs.3,10 and 17.

4. Preparing p-Anthraquino N-phenyl 3,4-selenadiazo Benzophenone Imine (IV)

An amount of (2 mmol) 0.725 g of N-phenyl 3,4-selenadiazo benzophenone imine was dissolved in 30 ml of acetonitrile and mixed with (2 mmol) 0.416 g of anthraquinone dissolved in 30 ml of acetonitrile and heated using reflux in a water bath for 3 hours. The solution was cooled and evaporated by a rotary evaporator and washed with small amounts of acetonitrile to obtain pure and shiny light-yellow crystals precipitate with an 64% yield and an M.P (melting point) of 118-208 °C. Rf value=0.85 (7:3) (Ethyl acetate\n-hexane). UV-visible spectra were recorded at 200-750 nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions with Λ max (215 nm, 230 nm,240 nm, 248 nm, 252 nm, 275 nm, 350 nm). FT-IR with KBr disk: υ(C–H) Aromatic = 3070 cm^{-1}, υ(C=N) Aromatic = 1639-1676 cm^{-1}, Ar. υ(C=O) = 1737-1795 cm^{-1}, υ (C=C) Aromatic = 1545-1589 cm^{-1}, υ(C–N) Ar. = 1330 cm^{-1}, Ar. υ(C-Se-N) = 3319 cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6) δ Ar. $_{13}$C-H, $_{15}$C-H (2H, m, δ 7.58-7.69), δ Ar. $_{14}$C-H, $_{16}$C-H $_{17}$C-H, (3H, m, δ 7.57-7.63), δ Ar. $_{20}$C-H, $_{21}$C-H, $_{19}$C-H, $_{22}$C-H, (4H, m, δ 7.57 -7.76), δ Ar. $_{30}$C-H, $_{31}$C-H, $_{32}$C-H, $_{33}$C-H, $_{34}$C-H, $_{35}$C-H$_{36}$C-H, $_{37}$C-H (8H, m, δ 7.85 -7.95) Ar. $_{23}$C-H (1H, d, δ 8.3); Ar. $_9$C-H, (1H, d, δ 8.26); Ar. $_8$C-H, (1H, d, δ 8.20); Ar. $_6$C-H, (1H, s, δ 8.09); as show in Scheme3, Table1,2 and 3, Figures.4,11 and 18.

5. Preparing Tetrachloro Benzoquino N-phenyl 3,4-selenadiazo Benzophenone Imine(V)

An amount of (2 mmol) 0.725 g of N-phenyl 3,4-selenadiazo benzophenone imine was dissolved in 30 ml of acetonitrile and mixed with (2 mmol) 0.491 g of Tetrachloro benzoquinone dissolved in 30 mL of acetonitrile and heated using reflux in a water bath for 3 hours. The solution was cooled and evaporated by a rotary evaporator and washed with small amounts of acetonitrile to obtain a pure and shiny dark brown crystal crystals precipitate with an 71% yield and an M.P (melting point) of 170-230 °C. Rf value=0.88 (7:3) (Ethyl acetate\n-hexane). UV-visible spectra were recorded at (200-750) nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions with Λ max 215 nm, 237 nm, 240 nm, 248 nm, 285 nm, 350 nm. FT-IR with KBr disk: υ(C–H) Aromatic = 3063 cm^{-1}, υ(C=N) Aromatic = 1639-1683 cm^{-1}, υ(C=O) Aromatic = (1768) cm^{-1}, Ar. υ (C=C) = 1570-1591 cm^{-1}, υ(C–N) Ar. = 1325 cm^{-1}, υ(C-Se-N) Aromatic = 3356 cm^{-1}, υ(C-Cl) Ar. = 550-880 cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6) were δ Ar. $_{13}$C-H(1H, d, δ 8.03), δ Ar. $_{14}$C-H, $_{15}$C-H, $_{16}$C-H (3H, m, δ 7.86-7.87), δ Ar. $_{17}$C-H, $_{20}$C-H, $_{21}$C-H(3H, m, δ 7.58-7.77), δ Ar. $_{23}$C-H (1H, d, δ 7.62); Ar. $_{19}$C-H, (1H, d, δ 7.9), $_{22}$C-H (1H, t, δ 7.59); Ar. $_9$C-H, (1H, d, δ 8.02); Ar. $_8$C-H, (1H, d, δ 8.01); Ar. $_6$C-H, (1H, s, δ 8.10); as show in Scheme3, Table1,2 and 3, Figuers.5, 12 and 19.

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6. Preparing 7,7,8,8-Tetracyano Quino Dimethane N-phenyl 3,4-selenadiazo Benzophenone Imine (VI)

An amount of (2 mmol) 0.725 g of N-phenyl 3,4-selenadiazo benzophenone imine was dissolved in 30 ml of acetonitrile and mixed with (2 mmol) 0.408 g of 7,7,8,8-Tetracyano quino dimethane dissolved in 30 ml of acetonitrile and heated using reflux in a water bath for 3 hours. The solution was cooled and evaporated by a rotary evaporator and washed with small amounts of acetonitrile to obtain a pure and shiny dark yellow crystal precipitate with an 71% yield and an M.P (melting point) of (149-260) C°. Rf value=0.92 (7:3) (Ethyl acetate\n-hexane). UV-visible spectra were recorded at 200-750 nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions with Λ max 210 nm, 220 nm, 225 nm, 245 nm, 250 nm, 365 nm, 400 nm. FT-IR with KBr disk: υ(C–H) Aromatic = 3051 cm^{-1}, υ(C=N) Ar. = (1651-1676) cm^{-1}, υ(C=C) Ar. = 1541 cm^{-1}, υ(C–N) Ar. = 1354 cm^{-1}, υ(C-Se-N) Ar. = 3138 cm^{-1}, υ(C≡N) Ar. = (2222) cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6): δ Ar. $_{13}$C-H, (1H, d, δ 8.01) δ Ar. $_{23}$C-H, $_{14}$C-H (2H, m, δ 7.86-7.88), δ Ar. $_{15}$C-H, $_{16}$C-H (2H, m, δ 7.72-7.76), δ Ar. $_{17}$C-H, $_{20}$C-H, $_{21}$C-H, (3H, m, δ 7.86 -7.88), δ Ar. $_{25}$C-H, $_{26}$C-H, $_{28}$C-H, $_{29}$C-H (4H, m, δ (7.88 -7.89), Ar. $_{22}$C-H, $_{19}$C-H, (2H, t, δ 7.60-7.63); Ar. $_9$C-H, (1H, d, δ 8.01); Ar. $_8$C-H, (1H, d, δ 8.02); Ar. $_6$C-H, (1H, s, δ 8.09); as show in Scheme3, Table1,2 and 3, Figures.6,13 and 20.

7. Preparing 1,4-Dihydroxyanthraquino N-phenyl 3,4-selenadiazo Benzophenone Imine (VII)

An amount of (2 mmol) 0.725 g of N-phenyl 3,4-selenadiazo benzophenone imine was dissolved in 30 ml of acetonitrile and mixed with (2 mmol) 0.48 g of 1,4-Dihydroxyanthraquinon dissolved in 30 ml of acetonitrile and heated using reflux in a water bath for 3 hours. The solution was cooled and evaporated by a rotary evaporator and washed with small amounts of acetonitrile to obtain a pure and shiny pink-yellow crystals precipitate with an 70% yield and an M.P (melting point) of 167-187 C°. Rf value=0.88 (7:3) (Ethyl acetate\n-hexane). The UV-visible spectra were recorded at (200-750) nm in solvent of DMSO, n-π* and π-π* are two different types of electronic transitions with Λ max (210 nm, 225 nm, 230 nm, 245 nm, 255 nm, 273 nm, 335 nm, 473 nm). FT-IR with KBr disk: υ(C–H) Ar. = 3061 cm^{-1}, υ(C=N) Ar. = 1629 cm^{-1}, υ(C=O) Ar.= 1691 cm^{-1}, υ(C=C) Ar. = (1539-1589) cm^{-1}, υ(C–N) Ar. = 1357 cm^{-1}, υ(C-Se-N) Ar.= 3210 cm^{-1}, υ (OH) Ar. = (3500-3600) cm^{-1}; Signals of ^{1}H-NMR (500 MHz-DMSO-d^6): δ Ar. $_{13}$C-H, $_{14}$C-H (2H, m, δ 7.49-8.02), δ Ar. $_{15}$C-H, $_{16}$C-H (2H, t, δ 8.02-8.03), Ar. $_{17}$C-H (1H, s, δ 8.31), δ Ar. $_{21}$C-H, $_{22}$C-H (2H, t, δ7.49-8.02), $_{19}$C-H, $_{23}$C-H, (2H, d, δ 7.57 -7.76), δ Ar. $_{27}$C-H, $_{28}$C-H, $_{34}$C-H, $_{35}$C-H$_{36}$C-H, $_{37}$C-H (6H, m, δ 8.30 -8.03) Ar. $_{20}$C-H (1H, d, δ 8.03); Ar. $_9$C-H, (1H, d, δ 8.31); Ar. $_8$C-H, (1H, d, δ 8.30); Ar. $_6$C-H, (1H, s, δ 8.32) δ Ar. $_{39}$O-H, $_{40}$O-H (2H, s, δ 12.7); as show in Scheme3, Table1,2 and 3, Figures.7,14 and 21.
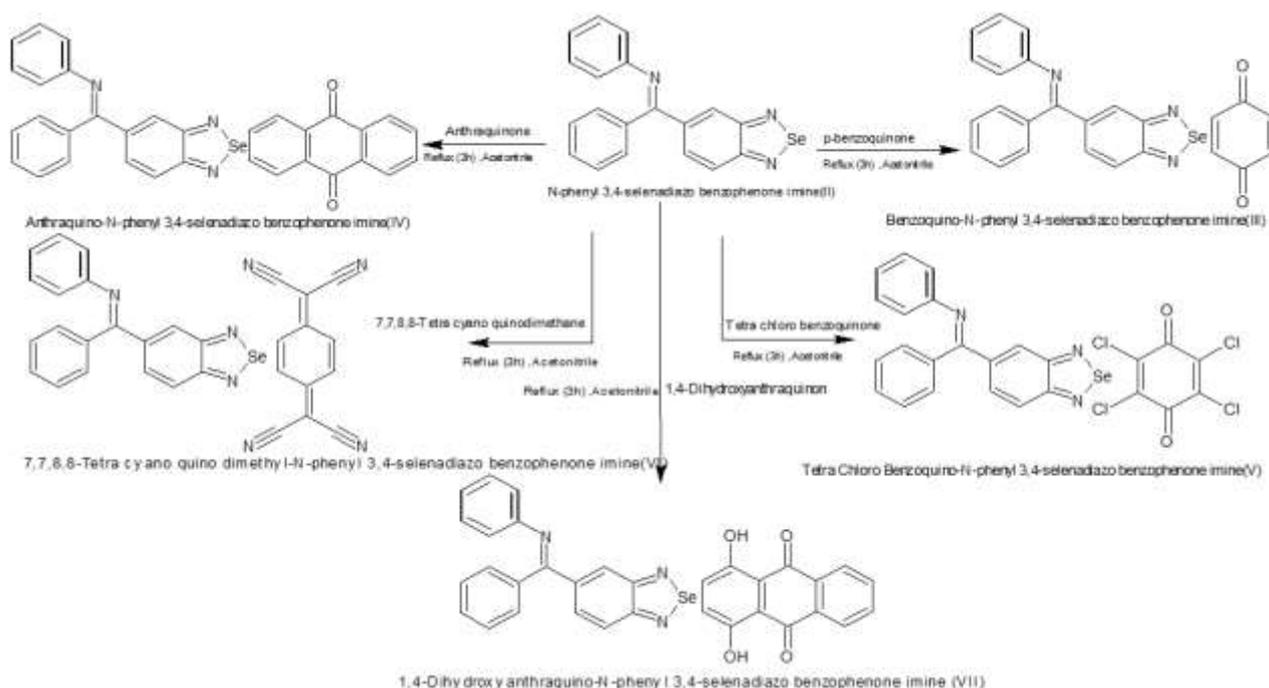
Scheme 3. Preparation of quino N-phenyl 3,4-selenadiazo Benzophenone Imine (compounds III, IV, V, VI, and VII)

Table 1. UV-visible (Á max nm) spectral data, yield, melting points, and Rf value of selected compounds.

Seq.	Compound	Á max of n-π* and π-π* transitions	yield of compound	melting point	Rf value
1	I	(225, 273, 355) nm	80%	95 °C.	0.78
2	II	(220, 233, 240, 243, 250, 270, 345) nm	76%	(105–110) C°.	0.93
3	III	(205, 230, 236, 270, 280, 355) nm	76%	107 C°	0.92
4	IV	(215, 230, 240, 248, 252, 275, 350) nm	64%	(118-208) C°	0.85
5	V	(215, 237, 240, 248, 285, 350) nm	71%	(170-230) C°	0.88
6	VI	(210, 220, 225, 245, 250, 365, 400) nm	71%	(149-260) C°	0.92
7	VII	(210, 225, 230, 245, 255, 273, 335, 473) nm	70%	(167-187) C°.	0.88

Table 2. The spectral FT-IR data of synthesized compounds.

functional group	Compounds						
	I	II	III	IV	V	VI	VII
Ar. C–H (cm⁻¹)	3061	3063	3063	3070	3063	3051	3061
Ar. (C=O) (cm⁻¹)	1649	-	1724 -1788	1737-1795	1768	-	1691
Ar. C=N(cm⁻¹)	1579-1600	1593-1637	1597-1639	1639-1676	1639-1683	1651-1676	1629
Ar. C=C(cm⁻¹)	1490-1500	1448-1556	1504-1575	1545-1589	1570-1591	1541	1539-1589
Aliphatic C=C(cm⁻¹)	-	-	-	-	-	1433	-
Ar. C-Se-N(cm⁻¹)	3248.54	3250	3259	3319	3356	31380	3210
Aliphatic C≡N(cm⁻¹)	-	-	-	-	-	2222	-
Ar. OH (cm⁻¹)	-	-	-	-	-	-	3500-3600
Ar. C-Cl(cm⁻¹)	-	-	-	-	550-880	-	-
Ar. C-N(cm⁻¹)	-	1325	1325	1330	1325	3354	1357

Table 3. The spectral¹H-NMR data of synthesized compounds.

Seq	compounds	synthesized compounds Structure	Signals of ¹H-NMR TMS= 0 ppm (DMSO-d₆)
1	I		δ Ar. $_{14}$C-H, $_{16}$C-H (2H, m, δ 7.52); Ar. $_{15}$C-H, $_{17}$C-H (2H, m, δ 7.74); Ar. $_{13}$C-H, (1H, t, δ 7.89); Ar. $_9$C-H, (1H, d, δ 7.90); Ar. $_8$C-H, (1H, d, δ 8.02); Ar. $_6$C-H, (1H, s, δ 8.11).
	II		δ Ar. $_{13}$C-H, $_{14}$C-H, $_{15}$C-H, $_{16}$C-H, $_{17}$C-H, $_{20}$C-H, $_{21}$C-H, $_{22}$C-H (8H, m, δ 7.5-7.7); Ar. $_{19}$C-H, $_{23}$C-H (2H, m, δ 8.2); Ar. $_9$C-H, (1H, d, δ 8.01); Ar. $_8$C-H, (1H, d, δ 8.03); Ar. $_6$C-H, (1H, s, δ 8.10)

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2 **III**

δ Ar. $_{13}$C-H, $_{14}$C-H (2H, m, δ 7.53), δ Ar. $_{15}$C-H, $_{16}$C-H (2H, m, δ 7.58), δ Ar. $_{17}$C-H, $_{19}$C-H, $_{20}$C-H, $_{21}$C-H, $_{22}$C-H, (5H, m, δ 7.53 -7.77), δ Ar. $_{25}$C-H, $_{26}$C-H, $_{28}$C-H, $_{29}$C-H (4H, m, δ 7.85 -7.90) Ar. $_{23}$C-H (1H, d, δ 7.52); Ar. $_9$C-H, (1H, d, δ 8.01); Ar. $_8$C-H, (1H, d, δ 8.02); Ar. $_6$C-H, (1H, s, δ 8.10)

3 **IV**

δ Ar. $_{13}$C-H, $_{15}$C-H (2H, m, δ 7.58-7.69), δ Ar. $_{14}$C-H, $_{16}$C-H $_{17}$C-H, (3H, m, δ 7.57-7.63), δ Ar. $_{20}$C-H, $_{21}$C-H, $_{19}$C-H, $_{22}$C-H, (4H, m, δ 7.57 -7.76), δ Ar. $_{30}$C-H, $_{31}$C-H, $_{32}$C-H, $_{33}$C-H, $_{34}$C-H, $_{35}$C-H $_{36}$C-H, $_{37}$C-H (8H, m, δ 7.85 -7.95) Ar. $_{23}$C-H (1H, d, δ 8.3); Ar. $_9$C-H, (1H, d, δ 8.26); Ar. $_8$C-H, (1H, d, δ 8.20); Ar. $_6$C-H, (1H, s, δ 8.09)

4 **V**

δ Ar. $_{13}$C-H (1H, d, δ 8.03), δ Ar. $_{14}$C-H, $_{15}$C-H, $_{16}$C-H (3H, m, δ 7.86-7.87), δ Ar. $_{17}$C-H, $_{20}$C-H, $_{21}$C-H (3H, m, δ 7.58-7.77), δ Ar. $_{23}$C-H (1H, d, δ 7.62); Ar. $_{19}$C-H, (1H, d, δ 7.9), $_{22}$C-H (1H, t, δ 7.59); Ar. $_9$C-H, (1H, d, δ 8.02); Ar. $_8$C-H, (1H, d, δ 8.01); Ar. $_6$C-H, (1H, s, δ 8.10);

5 **VI**

δ Ar. $_{13}$C-H, (1H, d, δ 8.01) δ Ar. $_{23}$C-H, $_{14}$C-H (2H, m, δ 7.86-7.88), δ Ar. $_{15}$C-H, $_{16}$C-H (2H, m, δ 7.72-7.76), δ Ar. $_{17}$C-H, $_{20}$C-H, $_{21}$C-H, (3H, m, δ 7.86 -7.88), δ Ar. $_{25}$C-H, $_{26}$C-H, $_{28}$C-H, $_{29}$C-H (4H, m, δ 7.88 -7.89), Ar. $_{22}$C-H, $_{19}$C-H, (2H, t, δ 7.60-7.63); Ar. $_9$C-H, (1H, d, δ 8.01); Ar. $_8$C-H, (1H, d, δ 8.02); Ar. $_6$C-H, (1H, s, δ 8.09);

6 **VII**

δ Ar. $_{13}$C-H, $_{14}$C-H (2H, m, δ 7.49-8.02), δ Ar. $_{15}$C-H, $_{16}$C-H (2H, t, δ 8.02-8.03), Ar. $_{17}$C-H (1H, s, δ 8.31), δ Ar. $_{21}$C-H, $_{22}$C-H (2H, t, δ7.49-8.02), $_{19}$C-H, $_{23}$C-H, (2H, d, δ 7.57 -7.76), δ Ar. $_{27}$C-H, $_{28}$C-H, $_{34}$C-H, $_{35}$C-H $_{36}$C-H, $_{37}$C-H (6H, m, δ 8.30 -8.03) Ar. $_{20}$C-H (1H, d, δ 8.03); Ar. $_9$C-H, (1H, d, δ 8.31); Ar. $_8$C-H, (1H, d, δ 8.30); Ar. $_6$C-H, (1H, s, δ 8.32) δ Ar. $_{39}$O-H, $_{40}$O-H (2H, s, δ 12.7)

Results and Discussion:

The current research included the synthesis of charge transfer complexes that were produced by N-phenyl 3,4-selenadiazo benzophenone imine[23] (prepared in the second step) by reacting N-phenyl 3,4-selenadiazo benzophenone imine [23] using acetonitrile as solvent and adding five types of different quinones (each quinone has a separate reaction) to obtain new charge transfer complexes compounds (III–VII). The transitions of n-π* typically experienced a significant shift in blue during synthesis complexes of charge-transfer. The

selenium atom is responsible for the deviating of the electron cloud around it and for a change in the evolution of the charge-transfer complexes. The bands of absorption shifted to shorter wave lengths when quinones' electron donors decreased the π-π^* and n-π^* transitions, chromophore group conjugate effects, increasing the required energy for transitions of π-π^* and n-π^*. Are provided in Figs. 1-7, as shown in Table1.
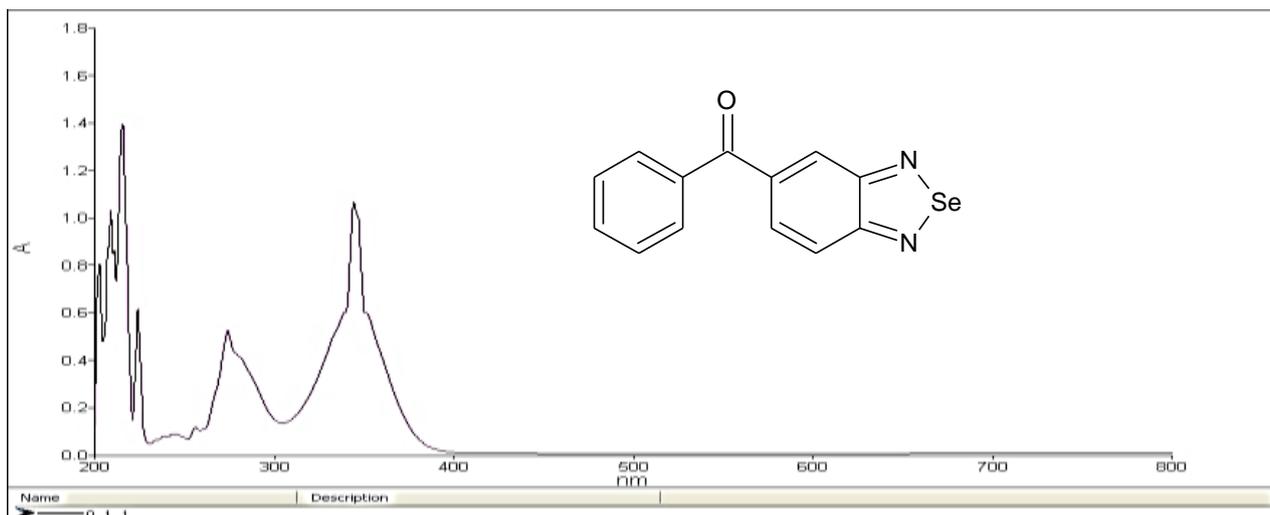
Figure 1. UV-Visible spectrum of compound (I).
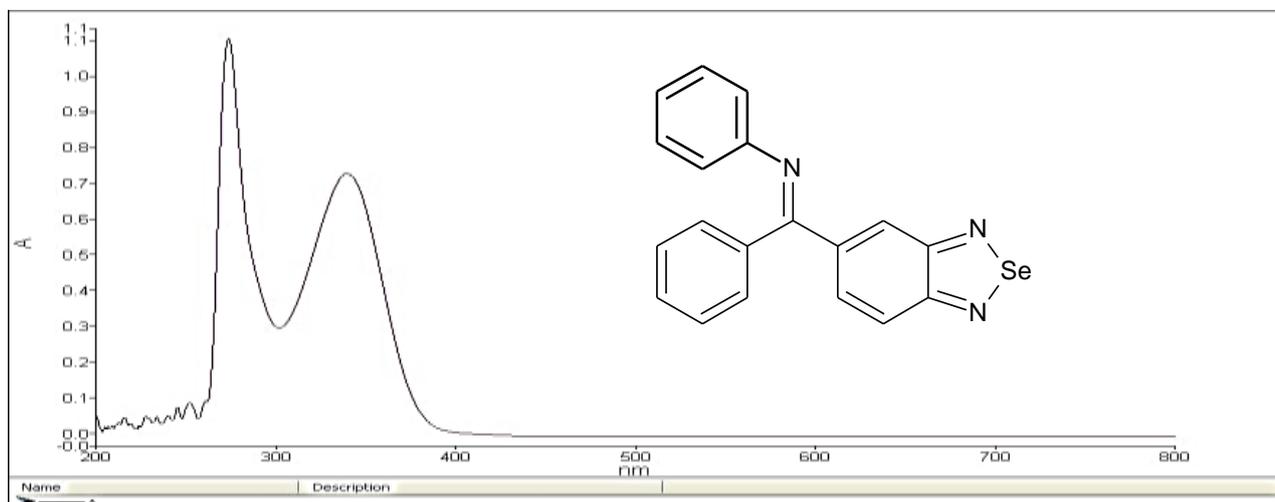
Figure 2. UV-Visible spectrum of compound (II).
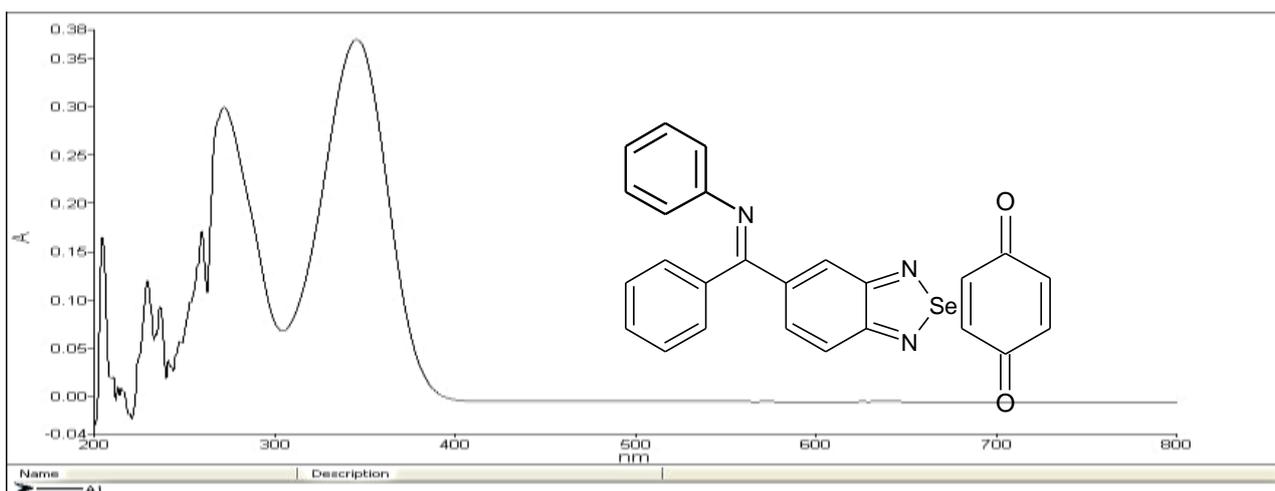
Figure 3. UV-Visible spectrum of compound (III).

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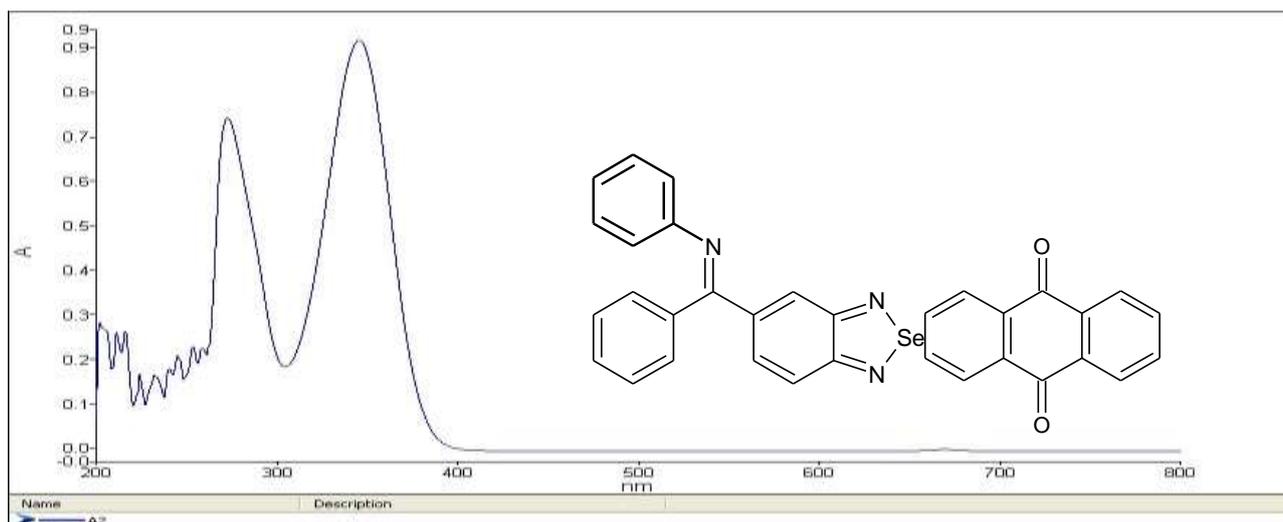
Figure 4. UV-Visible spectrum of compound (IV).
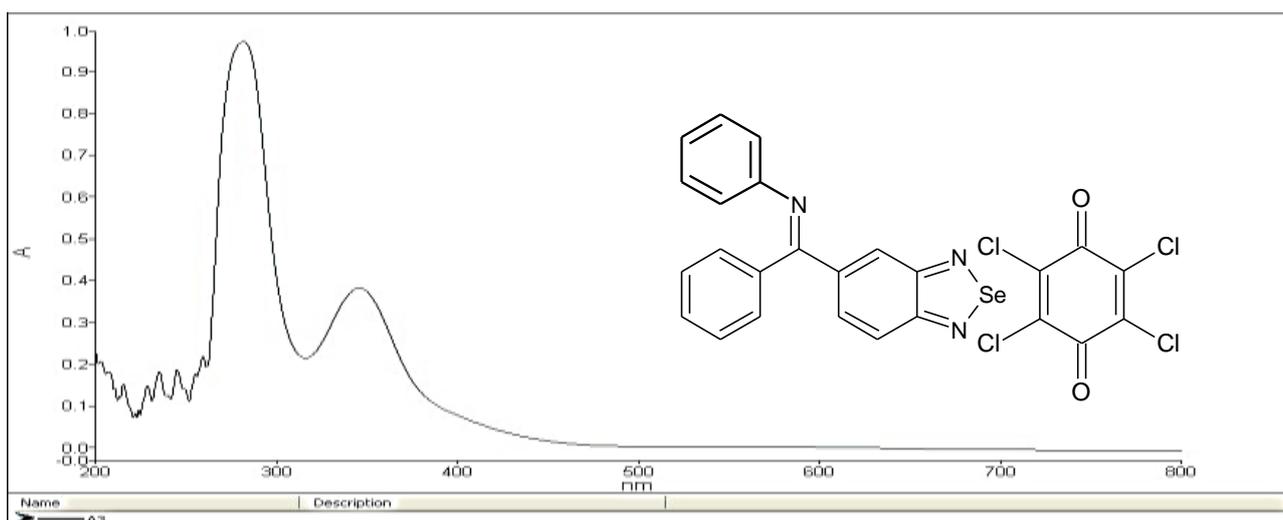
Figure 5. UV-Visible spectrum of compound (V).
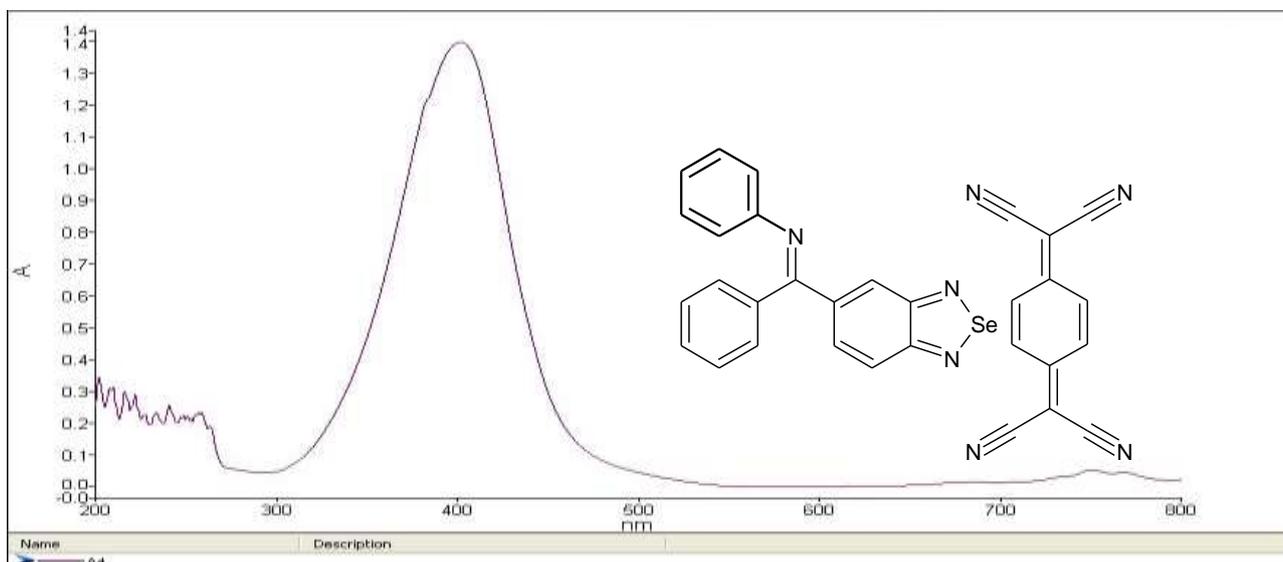
Figure 6. UV-Visible spectrum of compound (VI).
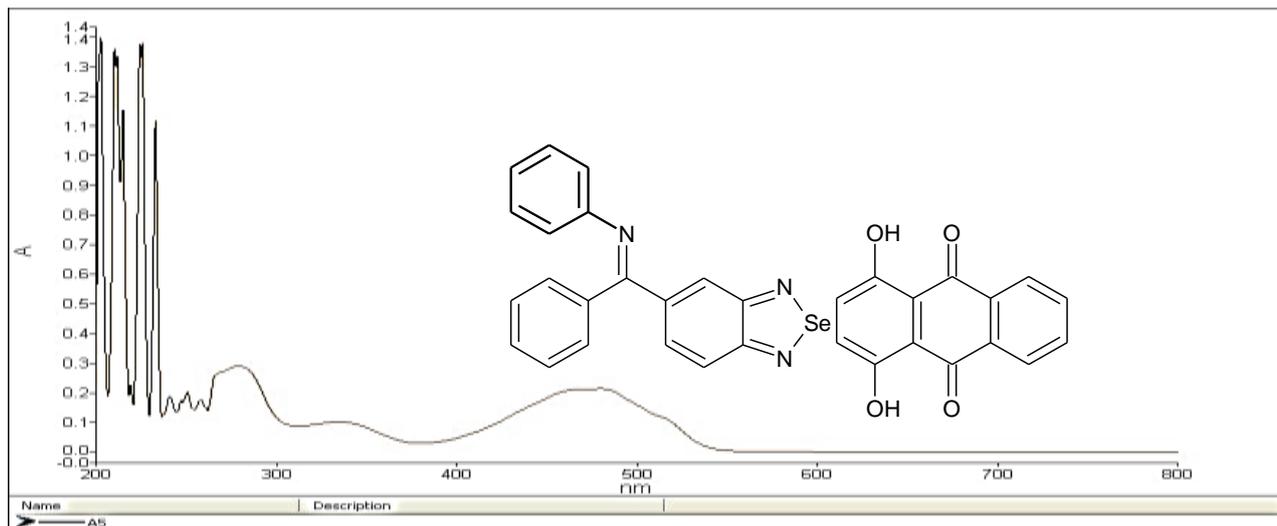
Figure 7. UV-Visible spectrum of compound (VII).
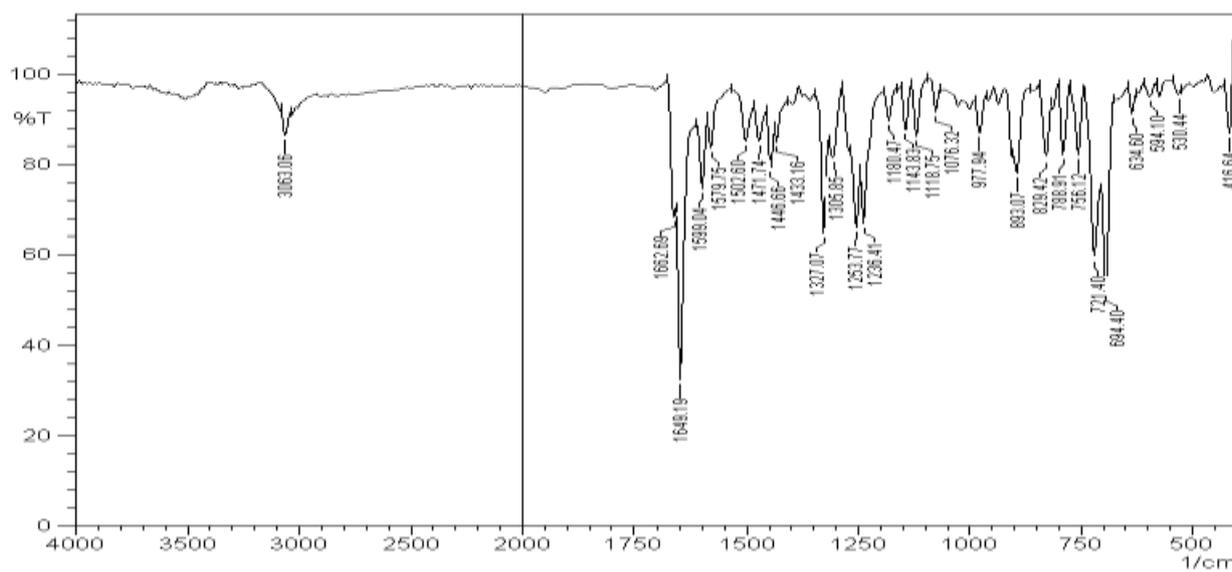
Figure 8. FT-IR spectrum of compound (I).
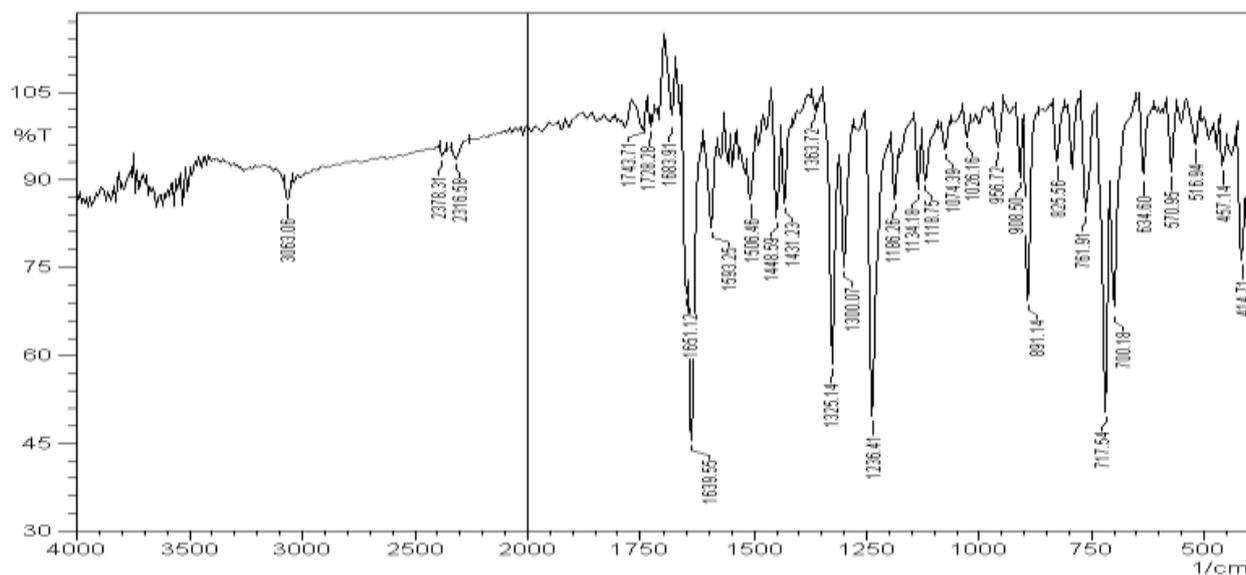
Figure 9. FT-IR spectrum of compound (II).
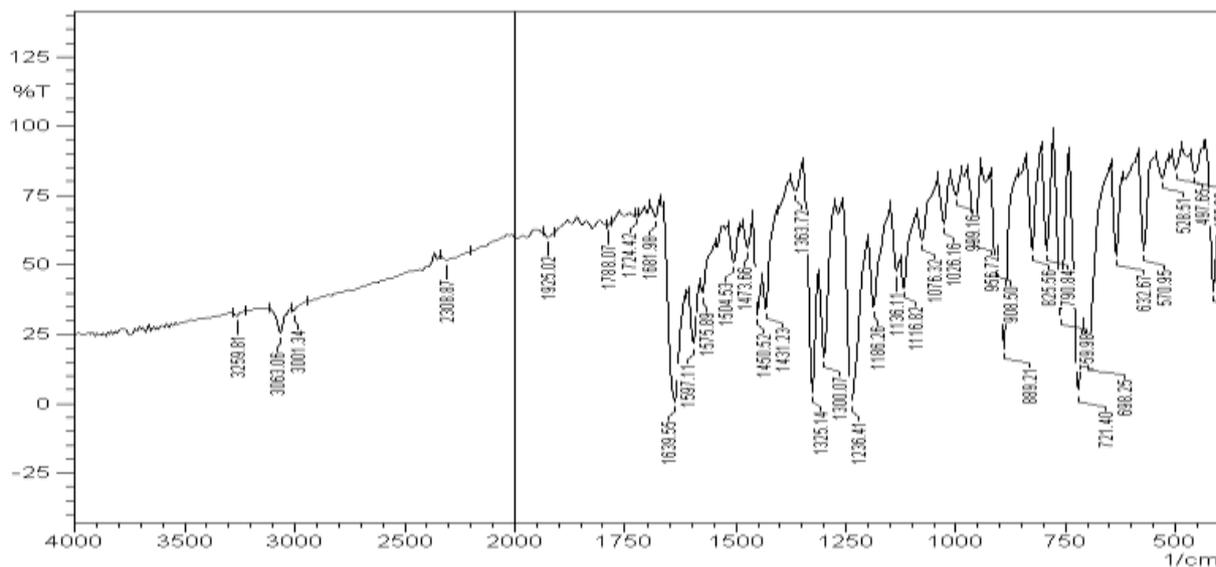
Figure 10. FT-IR spectrum of compound (III).
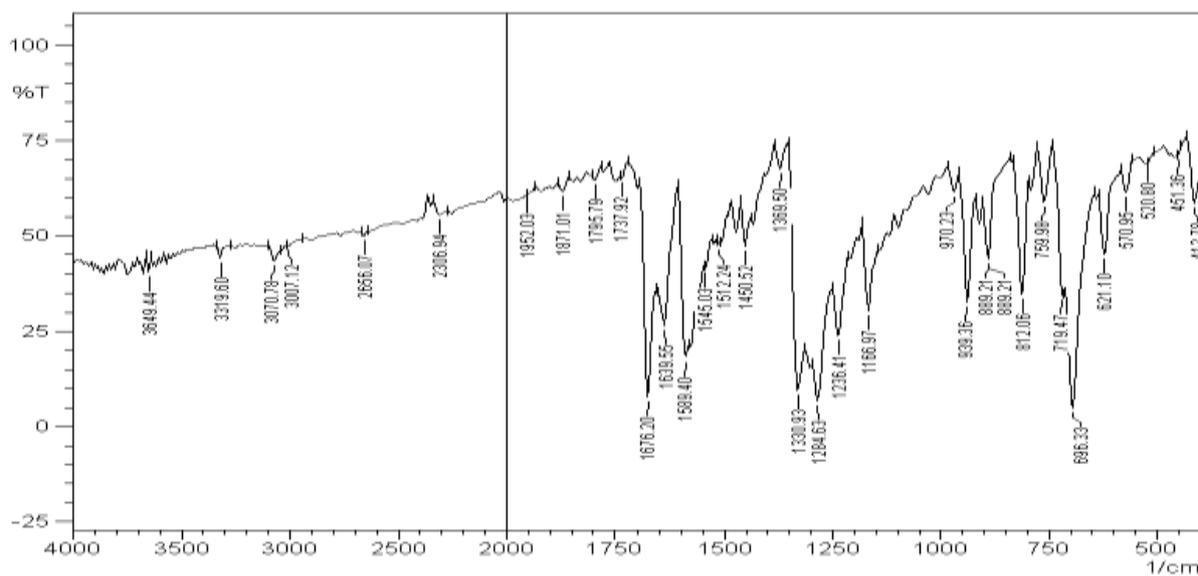
Figure 11. FT-IR spectrum of compound (IV).
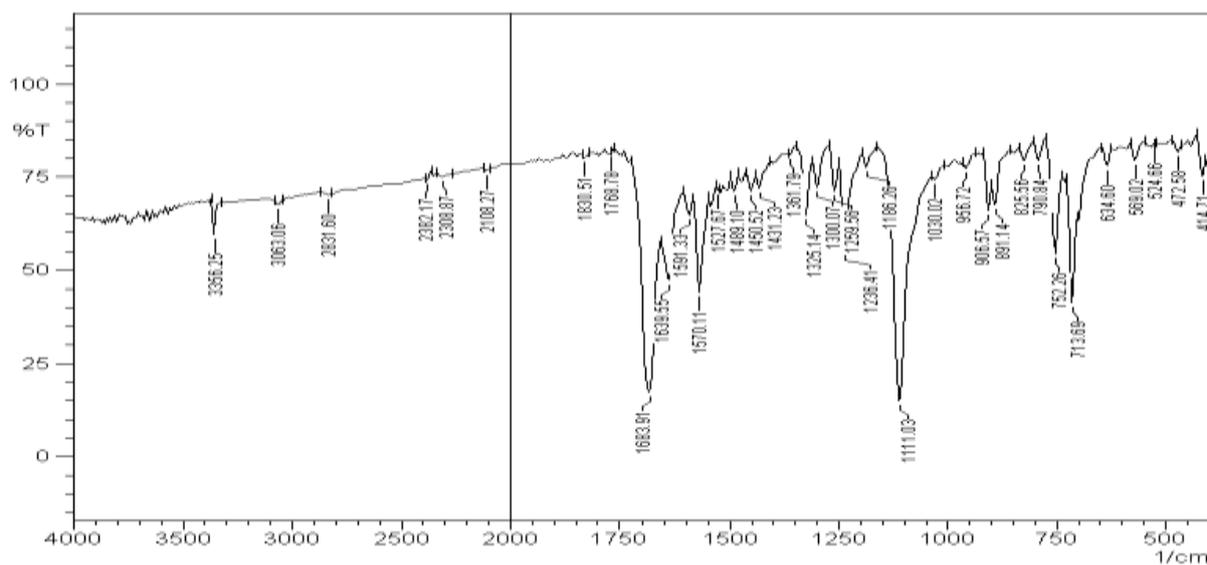
Figure 12. FT-IR spectrum of compound (V).
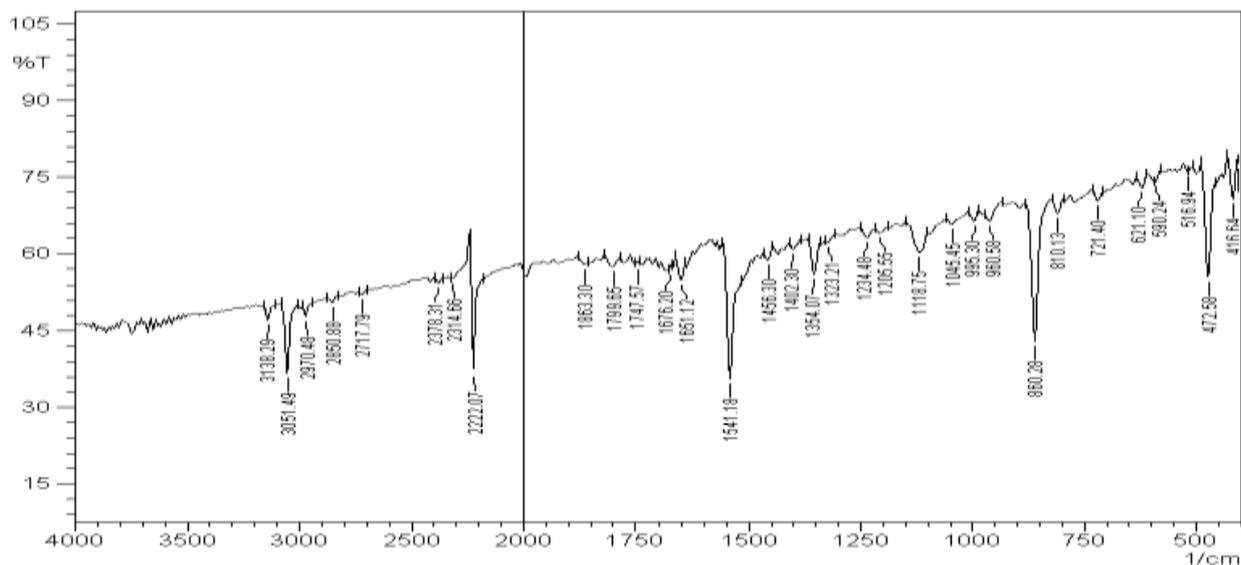
Figure 13. FT-IR spectrum of compound (VI).
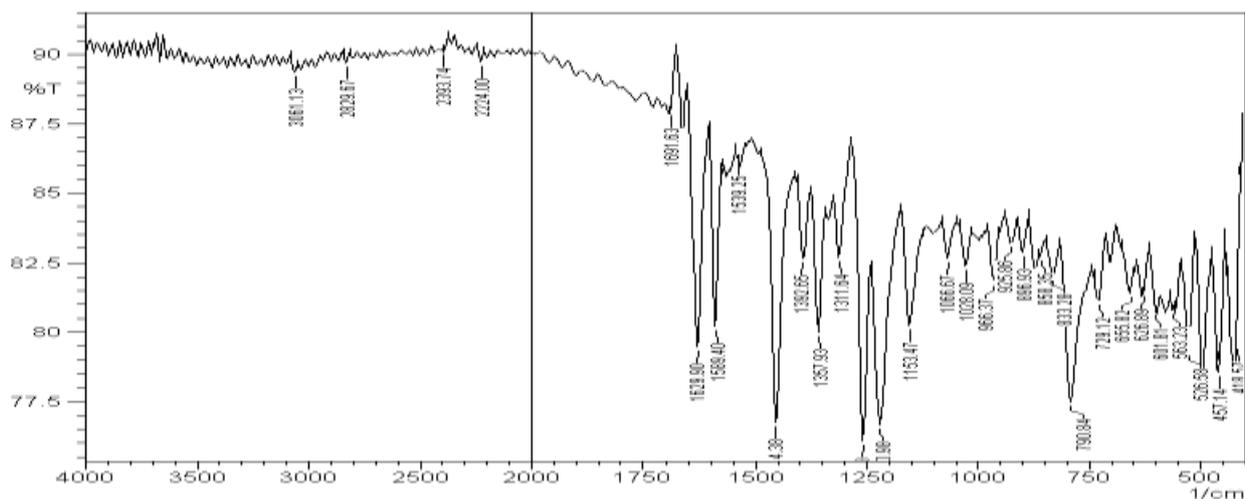
Figure 14. FT-IR spectrum of compound (VII).
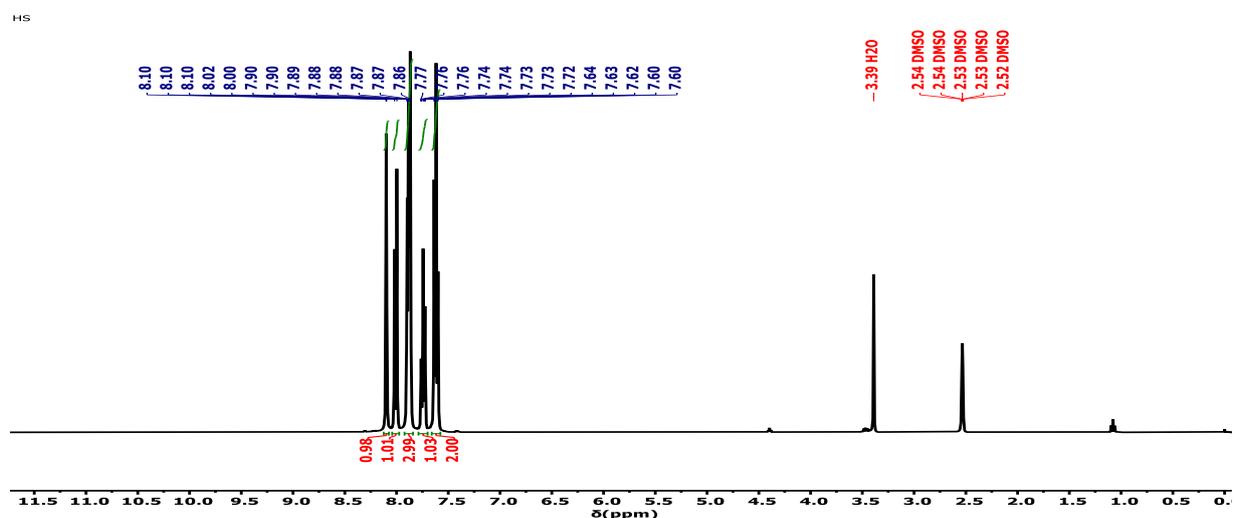
Figure 15. ¹H-NMR spectrum of compound 3,4-Selenadiazo benzophenone (I).
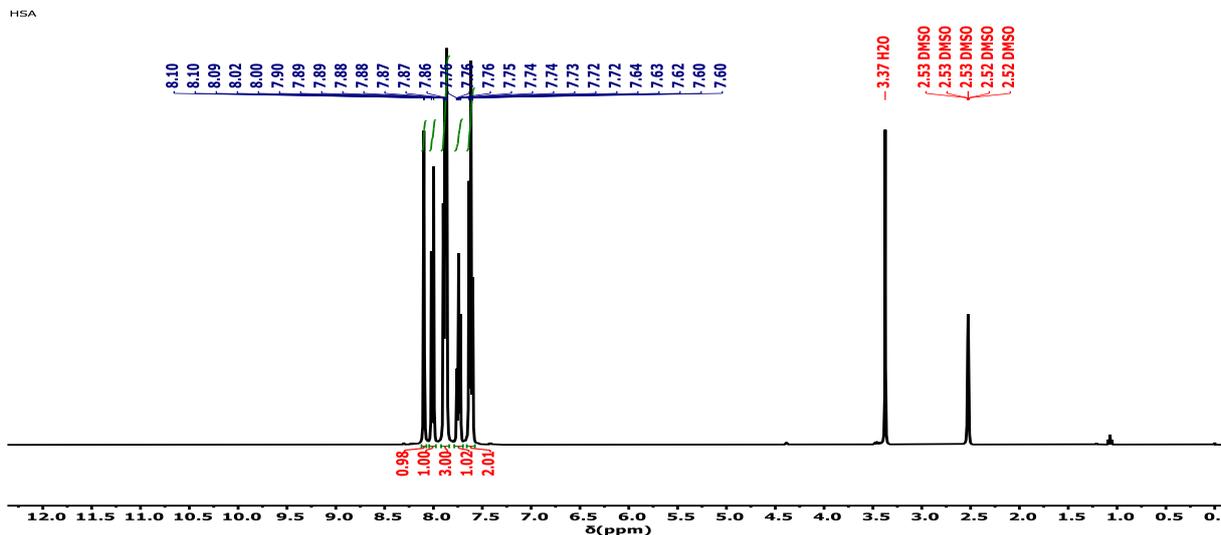
Figure 16. ^{1}H-NMR spectrum of compound (II).
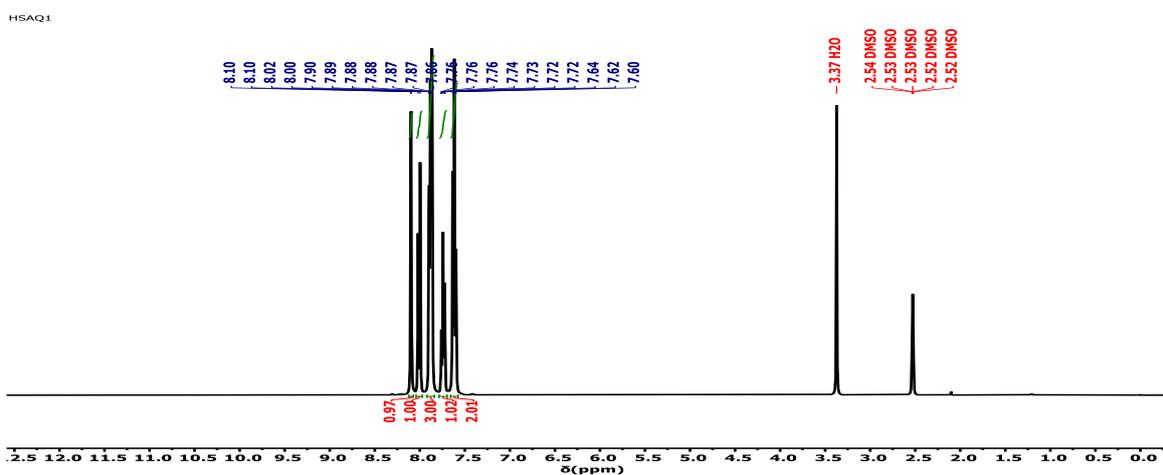
Figure 17. ^{1}H-NMR spectrum of compound (III).
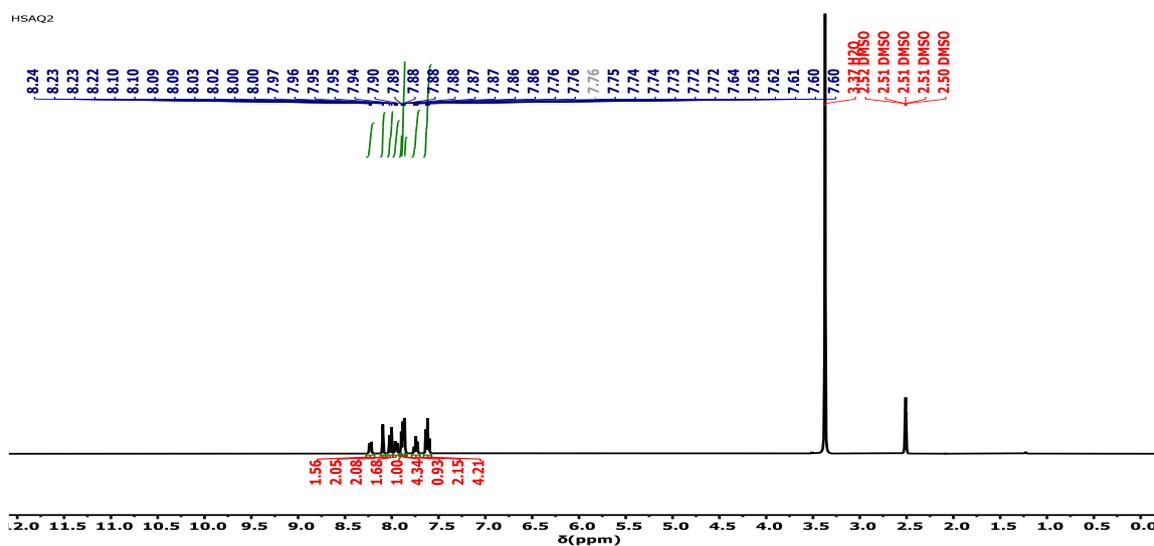
Figure 18. ^{1}H-NMR spectrum of compound (IV).

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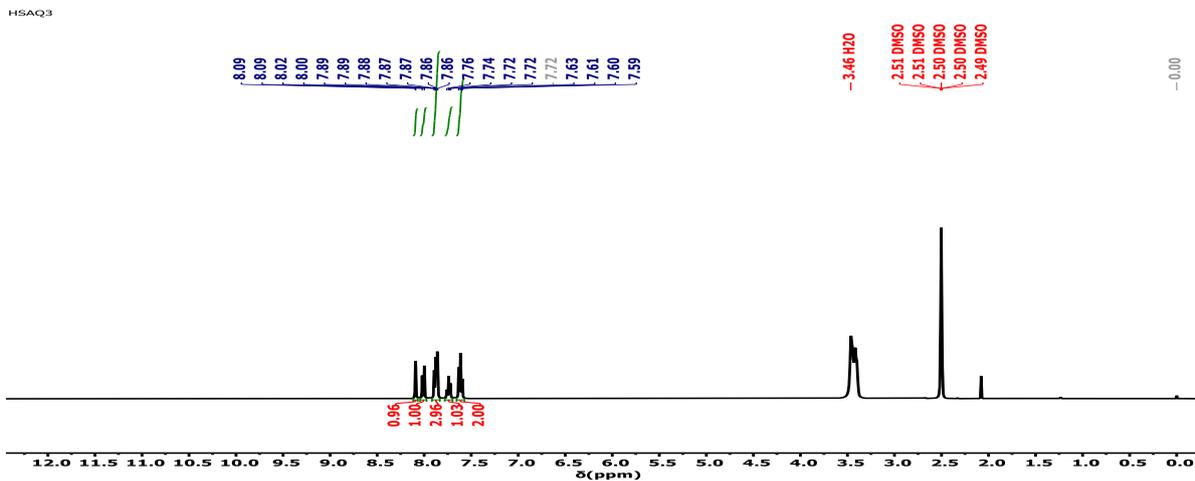
Figure 19. ¹H-NMR spectrum of compound (V).
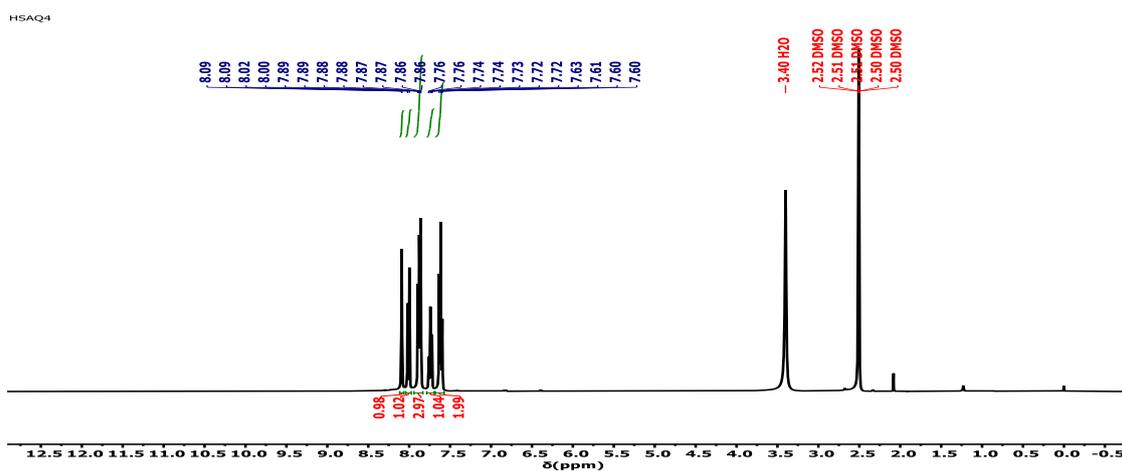
Figure 20. ¹H-NMR spectrum of compound (VI).
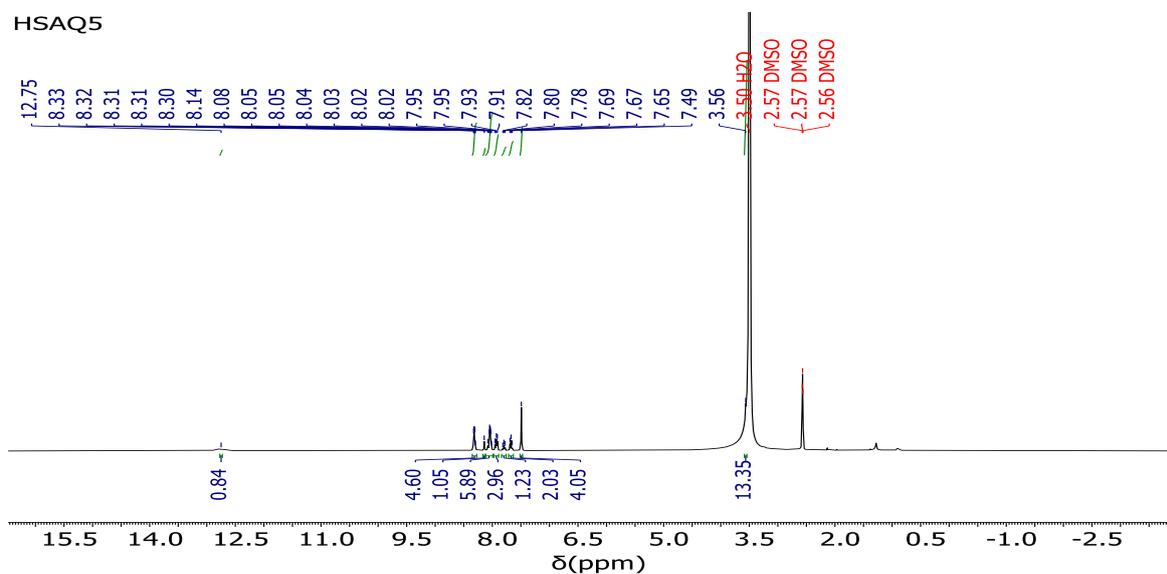
Figure 21. ¹H-NMR spectrum of compound (VII).

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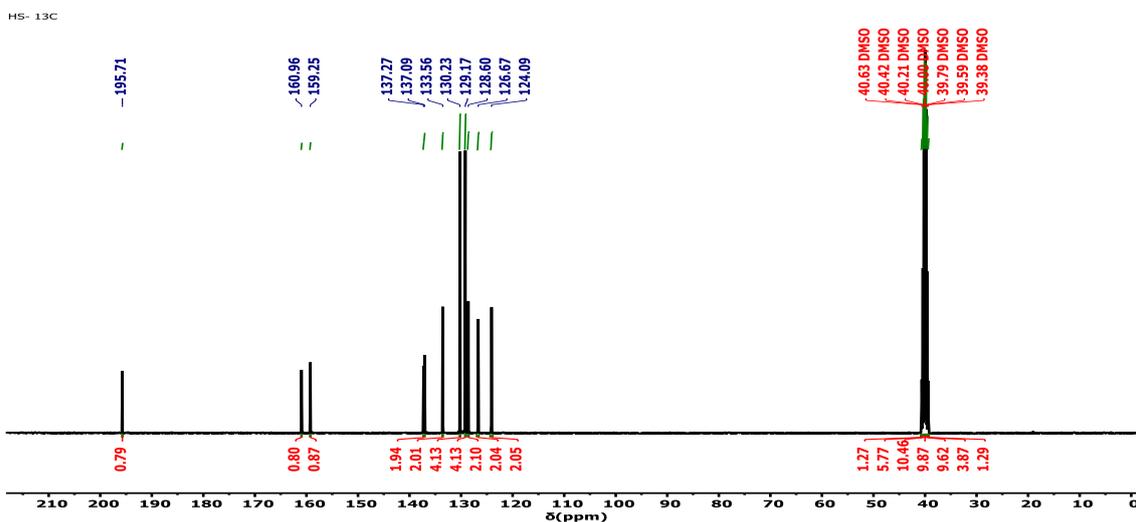
Figure 22. ¹³C NMR spectrum of compound 3,4-Selenadiazo benzophenone.
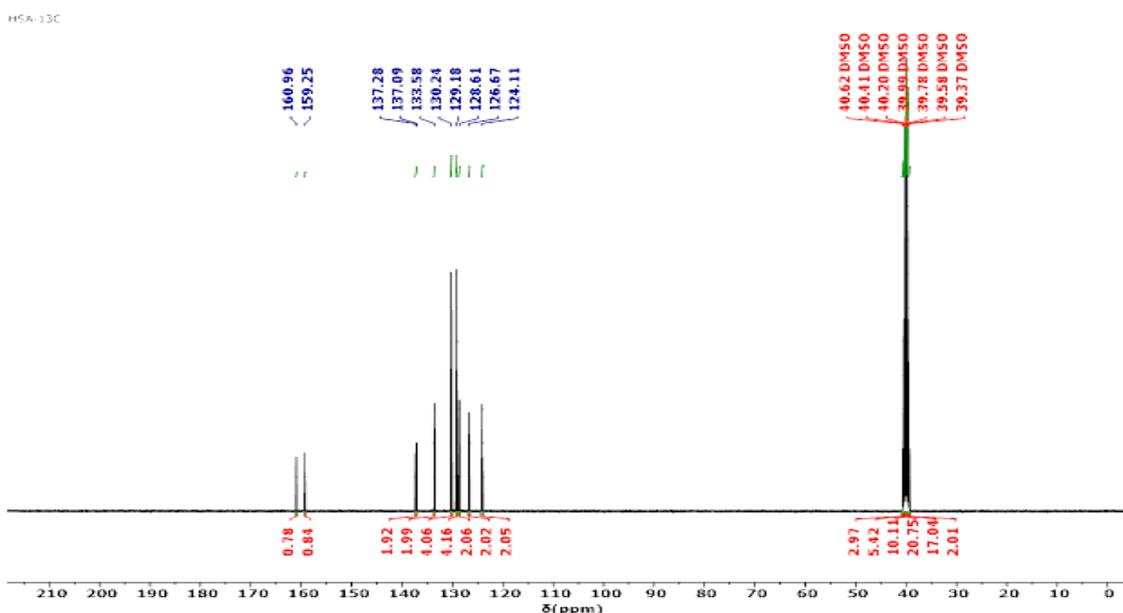
Figure 23. ¹³C NMR spectrum of compound N-phenyl 3,4-selenadiazo benzophenone imine.

UV-visible spectra were recorded at 200-750 nm in (DMSO) solvent, n-π* and π-π* are two different types of electronic transitions[24], are provided, such as Figs 1–7, as shown in Table 1. ʎ max for prepared complex compounds with a wavelength range of 205–473 nm. The infrared (IR) spectra of all synthesized complexes showed common characteristic bands and specific regions or other locations. The synthesized compounds suggested structures were verified by using the IR spectrum [25,26.] They are provided in Figs. 8–14 and Table 2. Ar. C-H appeared at 3051-3070 cm-1 for N-

phenyl 3,4-selenadiazo benzophenone imine and charge transfer complexes derivatives, while Ar. (C=O) appeared at 1649-1795 cm⁻¹, Ar. C=N at 1579-1683 cm⁻¹, whereas aliphatic C≡N at 2222 cm⁻¹, Ar. C=C at 1448-1591 cm⁻¹, Aliphatic C=C at 1433 cm⁻¹, Ar. C-Se-N at 3138-3356 cm⁻¹, Ar. O-H at 3500-3600 cm⁻¹, and Ar. C-l at 550-800 cm⁻¹. ¹H-NMR spectra of the compounds (I–VII) showed all the peaks as expected with explanations. Figs 15–21 and Table 3 show DMSO spectra for each selected compound.

Figure 24. Molecular structure Ball and tube model of compound (I).

Figure 25. Molecular structure Ball and tube model of compound (II).

Figure 26. Molecular structure Ball and tube model of compound (III).

Figure 27. Molecular structure Ball and tube model of compound (IV).

Figure 28. Molecular structure Ball and tube model of compound (V).

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Figure 29. Molecular structure Ball and tube model of compound (VI).
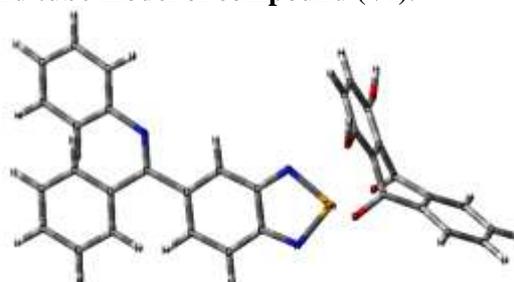
Figure 30. Molecular structure Ball and tube model of compound (VII).
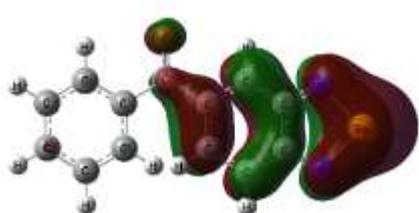
Figure 31. Mo. orbital (HOMO) of compound (I).   Figure 32. Mo. orbital (LUMO) of compound (I).
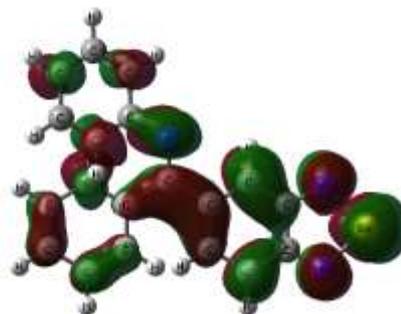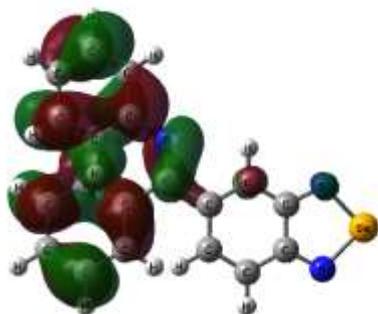
Figure 33. Mo. orbital (HOMO) of compound (II).   Figure 34. Mo. orbital (LUMO) of compound (II).
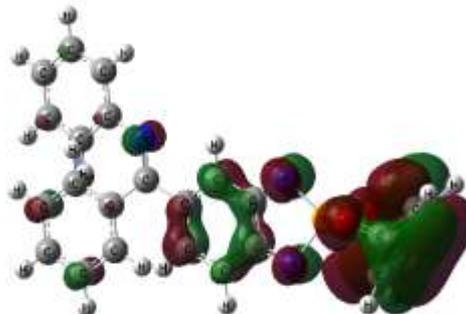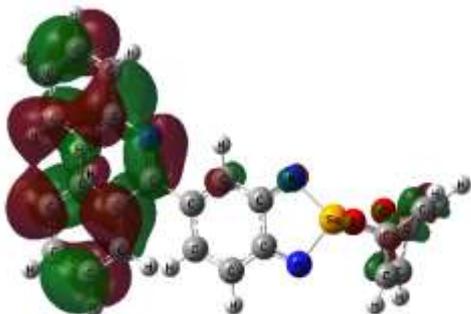
Figure 35. Mo. orbital (HOMO) of compound (III).   Figure 36. Mo. orbital (LUMO) of compound (III).
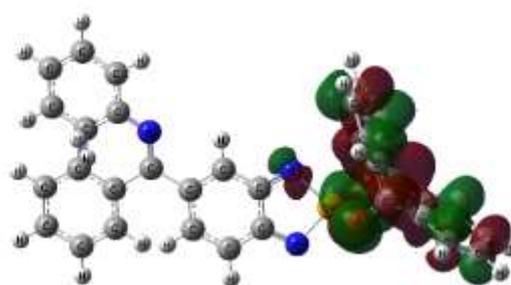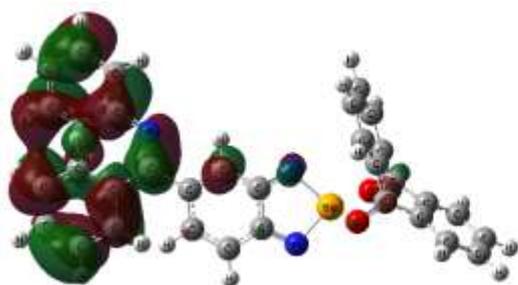
Figure 36. Mo. orbital (HOMO) of compound (IV).

Figure 37. Mo. orbital (LUMO) of compound (IV).
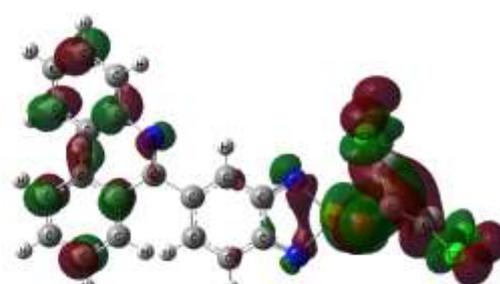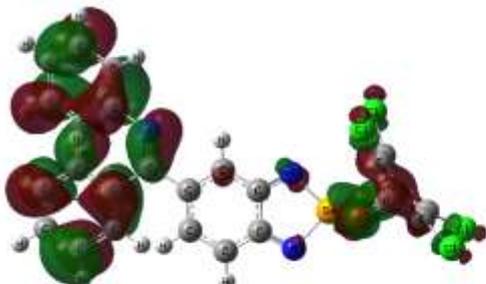
Figure 38. Mo. orbital (HOMO) of compound (V).

Figure 39. Mo. orbital (LUMO) of compound (V).
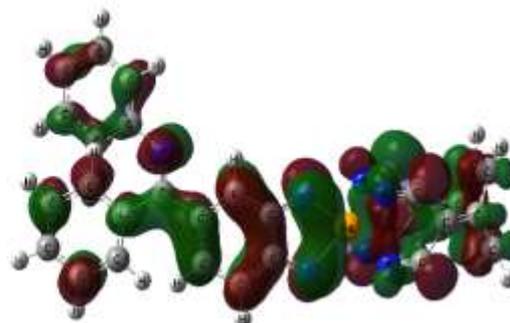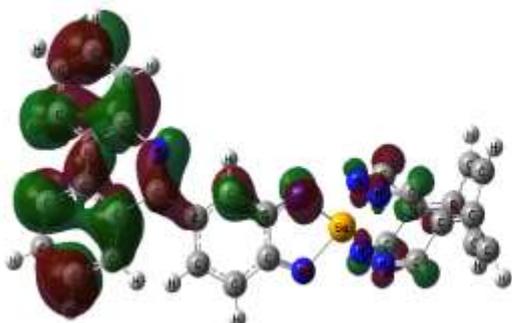
Figure 40. Mo. orbital (HOMO) of compound (VI).

Figure 41. Mo. orbital (LUMO) of compound (VI).
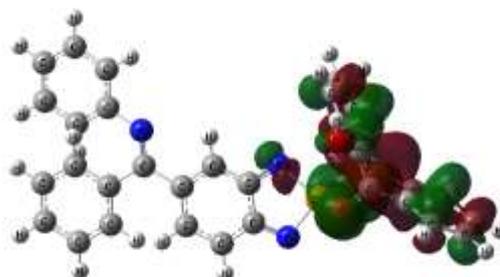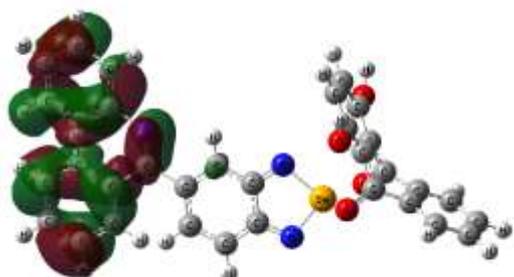
Figure 42. Mo. orbital (HOMO) of compound (VII).

Figure 43. Mo. orbital (LUMO) of compound (VII).

Computational Analysis

The charge-transfer complex compounds of N-phenyl 3,4-selenadiazo benzophenone imine under analysis were labeled as shown in Figs.24- 43. It was determined how well the method described the compound's properties in the gas phase. The functional theory of density (DFT) at hybrid functional (B3LYP), the levels of functional computational its combine between Parr's, and Lee, Yang correlation with exchange Becke's, was used to analyze the electronic characteristics and geometric structures of these compounds by all quantum calculations [27,28]. Using the basis of the set of 3–21G and the Gaussian (G09W) software, this method

described each atom [29]. Using estimated DFT-based descriptors, the compounds' reactivity and stability were assessed [30-33] through the mathematical relations as in the Eq.1, Eq.2, Eq.3 and Eq.4.

$$\mu = \left(\frac{\delta E}{\delta N}\right)_{V(\vec{r}),T} \quad \ldots \ldots \ 1$$

$$\eta = \frac{1}{2}\left(\frac{\delta^2 E}{\delta N^2}\right)_{V(\vec{r}),T} \quad \ldots \ 2$$

$$S = \frac{1}{2\eta} \quad \ldots \ 3$$

$$\omega = \frac{\mu^2}{2\eta} \quad \ldots \ 4$$

Where the μ = (chemical potential), η = (chemical hardness), S = (chemical softness), and ω = (electrophilicity), while E = (the total electron energy), N = (number of electrons), and V(r→) is (the external potential) respectively. The above global quantities were calculated by using two variations approaches; the first is a difference in a finite approximation, this is based on the changes in total electronic energy that occurs after the neutral molecule whenever an electron is added or removed. The energies of (HOMO) and (LUMO) different for molecules serve as the foundation for Koopman's theory[30,33,34]. Global quantities that are derivable from Eqs. 5 and 6 are approximated using finite differences.

$$\chi = \frac{(IP + EA)}{2} \quad \dots \quad 5$$

$$\eta = \frac{(IP - EA)}{2} \quad \dots \quad 6$$

But Koopman's theory, given by Eq.7, Eq.8.

$$\chi = \frac{(E_{HOMO} + E_{LUMO})}{2} \quad \dots \quad 7$$

$$\eta = \frac{(E_{HOMO} - E_{LUMO})}{2} \quad \dots \quad 8$$

The equilibrium geometries for all CT (charge-transfer) complex compounds in the gaseous phase were carefully tuned at level of the (DFT)[32] for theory using the functional of a (B3LYP,) in (G09W) and the basis standard established (3-21G) (see Figs. 24- 43). The energies of (HOMO) Molecular Orbital High Occupied and (LUMO) Molecular Orbital Low Unoccupied are the states of electrons, defining certain regions where atomic and molecular orbitals combine linearly, leading to the existence of electrons with quantized energy. The relationship between the energy band gap (Eg) Eq.9, Eq.6. and the difference in (LUMO) and (HOMO)[35]. The property of the Eg is essential in solids because it makes material prediction possible, if it is an insulator, semiconductor, or conductor. It depicts the difference in energy between the higher full energy level and the lower level of virtual energy.[36]. See Figs. (24– 43) and Table4.

$$Eg = E_{LUMO} - E_{HOMO} \quad \dots \quad 9$$

Electronegativity and Electrophilicity
The molecule's ability to take up electrons is measured by chemical electrophilicity, which is determined by chemical electrophilicity, which is dependent on chemical hardness and chemical potential, where hardness is resistance to deformation and change. On the other hand, electronegativity measures an atom's capacity to attract an electron density (a shared pair of electrons) towards itself. Calculating electrophilicity and electronegativity can be done using relationships in Eq.10, Eq.11.[22,30,31]; see Table 5.

$$\chi = \frac{(E_{HOMO} + E_{LUMO})}{2} \quad \dots \quad 10$$

$$\omega = \frac{\chi^2}{2\eta} \quad \dots \quad 11$$

Ionization Potential, and Electron Affinity
Measurement of the bond's strength is done via the ionization potential among an atom and an electron. It possesses the same amount of energy as what is needed to expel one electron from a neutral atom in the gas phase. When an atom takes an electron, energy is released, which is referred to as having a "electron affinity." It is the necessary energy to remove an electron from a negatively charged ion. This is consistent with Koopman's theory[28], as seen in Eq.12, Eq.13 and Table 6.

$$I.P = -E_{HOMO} \quad \dots \quad 12$$

$$E.A = -E_{LUMO} \quad \dots \quad 13$$

HSAB Principle (Acid Base Hardness Softness)
When utilized as acids and bases in chemistry, this principle describes how atoms or molecules behave. First, it must be shown that soft and hard acids are acceptors, whereas hard and soft bases are donors. Eq.14, Eq.15. are used to show both hardness and softness[37-39].

$$\eta = \frac{(IP - EA)}{2} \quad \dots \quad 14$$

$$\delta = \frac{1}{2\eta} \quad \dots \quad 15$$

Chemical softness and hardness are indicated, respectively, by the symbols (σ) and (η). based on Table 6.

Table 4. The electronic state compounds for charge-transfer complexes.

Compound,	HOMO, (eV)	LUMO, (eV)	Eg, (eV)
I	-6.43	-2.8848	3.545191
II	-3.35608	-3.01868	0.337404
III	-4.891	-2.7629	2.128094
IV	-3.06466	-2.56781	0.496855
V	-3.8894	-3.60152	0.287882
VI	-3.77403	-3.30357	0.470461
VII	-3.36479	-2.57842	0.786369

Table 5. Electronegativity and electrophilicity of compounds for the charge-transfer complex.

Compound	Electronegativity (eV) (X)	Electrophilicity (eV) (w)
I	-4.6574	-6.11853
II	-3.18738	-30.1105
III	-3.82695	-6.882
IV	-2.81624	-15.9628
V	-3.74546	-48.7299
VI	-3.5388	-26.6188
VII	-2.9716	-11.2294

Table 6. Ionization potential, electron affinity, softness, and hardness for charge-transfer complex compounds.

Compound	Ionization potential (eV) (I.P)	Electron affinity (eV) (E.A)	Softness (δ)	Hardness (η)
I	6.4299951	2.8848042	-1.7726	-0.28207
II	3.3560814	3.0186774	-0.1687	-2.96381
III	4.8909975	2.7629034	-1.06405	-0.4699
IV	3.0646623	2.5678077	-0.24843	-2.01266
V	3.8893974	3.6015156	-0.14394	-3.47365
VI	3.774027	3.3035661	-0.23523	-2.12558
VII	3.3647886	2.5784196	-0.39318	-1.27167

Conclusion:

The current work outlines simple and doable procedures for creating a variety of unique charge-transfer complex molecules. Compounds I, II, III, IV, V, VI, and VII were synthesized with a 64-80 percent yield rate. Results from the investigation of the FT-IR, 1 H-NMR, and UV-visible Spectrophotometer in the current study are consistent with those from earlier studies in these subjects. Verifying that the predicted structures for each of the synthesized molecules are accurate. Regarding the theoretic inquiry, it may be concluded that the DFT (density functional theory) to be used in the investigation is a reliable technique, as well as B3LYP functional is an appropriate and effective method function to analyze the electronic properties of these molecular structures. The testing results were consistent with the 3-21G's geometrical characteristics (d, p). The electronic properties for compounds of charge-transfer complex are investigated in this work utilizing the density functional theory (DFT) method, together with geometry optimization using the functionals of B3LYP.

Total energies in addition to geometric structures (donor and acceptor,) systems showed how extremely stable the structures are. Additionally, as compared to other systems, the donor-acceptor system has a higher reactivity and an average polarizability. As a result of the study's findings, we are now able to choose the kind of bridge that will work with acceptor and donor to determine the physical characteristics of the acceptor, bridge, and donor.

Authors' declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Thi-Qar.

Authors' Contribution Statement:

H. Sh. M. contributed in the design, acquisition of data, analysis, and the interpretation of the results. N. H. Al. contributed in the conception of the idea of the research, drafting the manuscript, revision and proofreading.

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تحضير، تشخيص واجراء دراسة نظرية لمعقدات انتقال الشحنة الجديدة المشتقة من N – فنيل -3,4- سيلينا داي ازو بنزو فينون امين

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الخلاصة:

في الدراسة الحالية، تم استخدام طريقة مباشرة لإنشاء سلسلة جديدة من معقدات نقل الشحنة من المواد الكيميائية ذات حصيلة جيدة، حيث تم إنتاج مركبات جديدة لمعقدات نقل الشحنة من خلال مفاعلة كينونات مختلفة كلا على حدة مع N- فنيل -3,4- سيلينا داي ازو بنزو فينون امين في مذيب الأسيتونيتريل بنسبة 1: 1 مول وباستخدام تقنيات التحليل المعروفة مثل الأشعة فوق البنفسجية ، والأشعة تحت الحمراء ، و-C^{13}, H^1 NMR، حيث تم تحديد جميع المواقع الفعالة للمركبات الناتجة حيث وجد انها تطابق نتائج التحليل للتراكيب الكيميائية المقترحة للمركبات المحضرة. بالإضافة الى ذلك تم استخدام نظرية الكثافة الوظيفية DFT لتحليل التركيب الجزيئي لمعقدات نقل الشحنة الناتجة من خلال استخدام برنامج الكاوسيين، حيث تم اكتشاف فجوة الطاقة الناشئة وأسطح HOMO و LUMO خلال عملية التحسين الهندسي باستخدام المجموعة الأساسية المكونة من 21G–3 من الهياكل الهندسية. كذلك تم تقييم الهندسة الجزيئية وخطوط المحيط للمركبات ذات معقدات نقل الشحنة أثناء التحسين الهندسي. كما تم التحقيق أيضًا في الذرات المستقبلة والمانحة لمعقدات نقل الشحنة الناتجة من خلال مقارنة طاقات HOMO للمواد الكيميائية في معقدات نقل الشحنة. كذلك، تم حساب ودراسة الحالة الارضية، والكهروسالبية، وجهد التأين، والكهروموجبية، والألفة الكهربية.

الكلمات المفتاحية : معقدات نقل الشحنة، كينونات مختلفة، فجوة طاقة، طاقات الهومو، N-فنيل-3,4- سيلينا داي ازو بنزو فينون امين.