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Simulation Study of Structural and Electronic Properties for Adducts complexes of Bis(Acetylacetonato)oxoVandium (IV) with 4-(*Para*-substituted phenyl)-1,2,3-Selenadiazole

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Abstract. A series of 4-(*para*-substituted phenyl)-1,2,3-selenadiazole adducts of $[VO(acac)_2]$ were studied by density functional theory (DFT) calculations. The 4-(*para*-substituted phenyl)-1,2,3-selenadiazole molecules have been selected to be bound with vanadium atom in $[VO(acac)_2]$ through Se, N2 and N3. The resulting adducts have been investigated in two geometries (*cis* and *trans*) in order to show the effect of such structural change on the electronic properties of the studied adducts. The optimized geometries, (binding and reorganization) energies and the spatial distribution of the highest molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the adducts are presented and discussed.

1. Introduction

Coordination complexes are of great significance in different fields due to their presence in many shapes and structures. There are numerous examples of coordination complexes in biochemistry field. For example, the iron, magnesium, cobalt and copper coordination complexes are demonstrated by hemoglobin, chlorophyll, Vitamin B-12 and hemocyanin respectively [1-4].

The Vanadyl moiety in coordination complexes has been extensively studied. Bis(acetylacetonato)oxidovanadium (IV), or $[VO(acac)_2]$, is one of the most important vanadium complexes [5]. X-ray diffraction studies on the $[VO(acac)_2]$ complex clearly show the existence and stability of VO^{+2} entity in the solid state. The geometry of complex demonstrates as an almost square pyramidal geometry [6]. Many applications have been demonstrated for the $[VO(acac)_2]$ complex. It has been used as the vanadium precursor for the preparation of different vanadium compounds [7-9] and also it has been used as a catalyst precursor in organic reactions [10-12]. Furthermore, Vanadium complexes show a wide variety of biological applications, and numerous complexes have been investigated as anti-parasitic, spermicidal, antiviral, anti-HIV, anti-tuberculosis, and antitumor agents [13].

Organo heterocyclic compounds of selenium which containing nitrogen such as selenirenes, selenophenes, selenadiazoles, selenatriazoles and benzisoselanazolones can have many biological effects. Among such features they are active immunostimulants, inhibitors of enzymes, antioxidants, anti-inflammatory, antitumor, antiviral and antimicrobial agents [14].

Bis(acetylacetonato)oxidovanadium(IV), or $[VO(acac)_2]$ is known to interact with various ligand containing donor atoms like N, P, O, S and Se to form adduct compounds. Although some vanadium-chalcogene complexes have been synthesized and characterized, only very few examples with analogous organo selenium derivatives as ligands have been described [15-18].

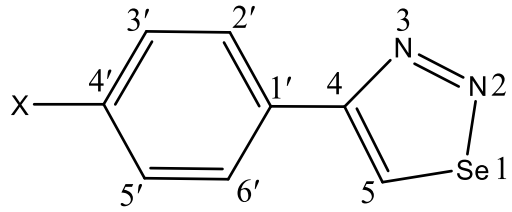
In this work, a series of 4-(*para*-substituted phenyl)-1,2,3-selenadiazole adducts of $[VO(acac)_2]$ have been investigated theoretically in order to show the effect of such structural change on the structural and electronic properties of the adducts.

2. Computational Methods

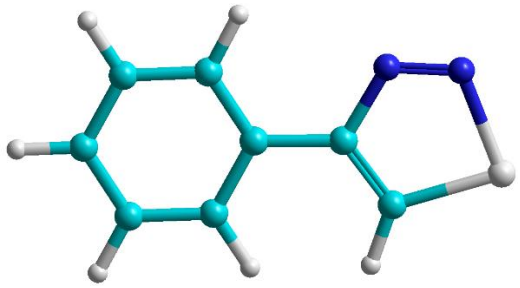
The calculations presented in this paper have been carried out by using hyperchem program 7.5 [19]. The geometry of the 4-(*para*-substituted phenyl)-1,2,3-selenadiazole ligands were optimized by carrying out the semiempirical molecular orbital theory at the PM3 level [20], using the restricted Hartree–Fock (RHF) procedure [21]. The Polak–Ribier algorithm [22] was used for the optimization, with the termination condition being a root mean square (RMS) of <0.001 kcal/mol. Further, Geometry optimization was done by performing the B3LYP/3-21G theory method [23-25]. Concerning the adduct molecules, the initial geometry optimization carried out with the molecular mechanics (MMC) force field [26-27], where the lowest energy conformations are obtained. Further, Geometry optimization was done was done by performing the B3LYP/STOG and B3LYP/3-21G theory methods. All calculations have been done on Pc, Intel(R) Core(TM) i3-3220 CPU @ 3.30GHz. Due to computational limitations and the large size of the studied adduct molecules, we were unable to achieve higher level optimizations on the adducts molecules.

3. Result and discussion

Scheme 1 shows the 4-(*para*-substituted phenyl)-1,2,3-Selenadiazole ligands. These ligands have been investigated theoretically to study their structural and electronic properties. Table 1 shows the calculated proton affinities of the substituted ligands according to semiemperical PM3 and BLYP/3-21G levels, the highest occupied and the lowest unoccupied molecular orbital energies (HOMO and LUMO respectively), their calculated hardness (1/2 the HOMO-LUMO gap). The values of hardness can give an information about the molecules if they are soft or hard, where the molecules which have a large HOMO-LUMO gap are hard while the molecules which have a small HOMO-LUMO gap are soft [28]. It can be seen clearly that electron-donating and electron-releasing groups have small effects on the hardness values for the calculations methods. For the PM3 calculation the trend of hardness of the substituted 1,2,3-selenadiazole ligands decrease in the order CF_3>H>Br>F>CN>CH_3>Cl>OCH_3>Ph>NH_2; while for BLYP/3-21G the hardness decrease in the order H>CF_3>CN>F>CH_3>Cl>Br>OCH_3>Ph>NH_2.



X= H, CH_3, Ph, NH_2, OCH_3, F, Cl, Br, CF_3, CN



Scheme 1. The general structure of 4-(*para*-substituted phenyl)-1,2,3-selenadiazole molecules (left) and optimized molecular structure of 4- phenyl-1,2,3-selenadiazole molecules (right)

The values of partial charges of selenium and nitrogen atoms are also given in Table 1. For both type of calculations, selenium atom indicates a positive charge. The Positive charge on the selenium atom should considerably decrease their base strengths electrostatically. Nitrogen is a better donor atom than Se. N2 atom possess negative charge vary from -0.092 to -0.085 and from -0.302 to -0.297 according to PM3 and BLYP/3-21G calculations respectively. N3 atom possess positive charge vary from 0.097 to 0.092 and negative charge vary from -0.294 to -0.272 according to PM3 and BLYP/3-21G calculations respectively.

Table 1. Selected calculated energy, hardness and parial charges of the 4-(*para*-substituted phenyl)-1,2,3-selenadiazole ligands according to semiempirical PM3 and BLYP/3-21G calculation.

X	Methods	E_{HOMO} eV	E_{LUMO} eV	Hardness eV	Mulliken charge			PA[a] (kcal/mol)	
					Se	N2	N3	N2	N3
H	PM3	-9.357	-1.280	4.039	0.158	-0.090	0.097	172.90	178.20
	3-21G	-6.222	-1.455	2.384	0.671	-0.296	-0.271	197.92	215.29
CH_3	PM3	-9.198	-1.251	3.974	0.156	-0.090	0.097	173.82	179.24
	3-21G	-6.009	-1.379	2.315	0.667	-0.297	-0.273	199.88	217.47
Ph	PM3	-8.921	-1.347	3.787	0.158	-0.090	0.096	174.21	181.78
	3-21G	-5.802	-1.750	2.026	0.652	-0.297	-0.289	201.11	220.32
NH_2	PM3	-8.226	-1.038	3.594	0.146	-0.092	0.092	178.57	185.30
	3-21G	-4.990	-1.327	1.832	0.630	-0.302	-0.294	194.33	209.03
OCH_3	PM3	-9.00	-1.221	3.890	0.155	-0.090	0.095	174.63	180.08
	3-21G	-5.655	-1.316	2.170	0.664	-0.297	-0.274	194.19	211.77
F	PM3	-9.444	-1.433	4.006	0.165	-0.087	0.095	170.76	175.57
	3-21G	-6.166	-1.529	2.319	0.675	-0.296	-0.273	195.86	212.71
Cl	PM3	-9.250	-1.395	3.928	0.163	-0.088	0.096	171.95	177.07
	3-21G	-6.253	-1.638	2.308	0.679	-0.294	-0.272	198.64	215.42
Br	PM3	-9.470	-1.433	4.019	0.165	-0.088	0.097	171.09	176.15
	3-21G	-6.141	-1.595	2.273	0.679	-0.295	-0273	197.83	214.86
CF_3	PM3	-9.810	-1.674	4.068	0.175	-0.085	0.098	167.68	172.28
	3-21G	-6.608	-1.884	2.362	o.690	-0.293	-0.269	195.46	212.17
CN	PM3	-9.654	-1.656	3.999	0.173	-0.086	0.097	168.50	173.19
	3-21G	-6.668	-2.031	2.319	0.710	-0.305	-0.282	190.62	207.06

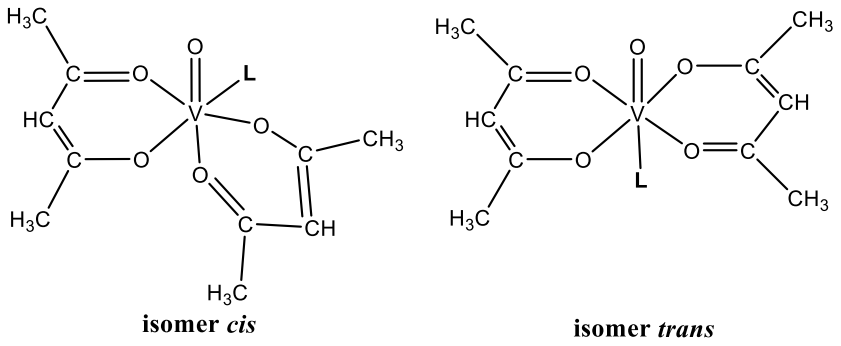
[a] PA are the values of ΔH and ΔE for PM3 and 3-21G calculations respectively for the reaction:
$BH^+ \longrightarrow B + H^+$(B selenadiazole)

The electron-releasing and electron-withdrawing effects of substituted groups are not reflected very well on the charges of both nitrogen and selenium atoms. The values of calculated proton affinity for N2 and N3 atoms are listed in Table 1. According to the PM3 and BLYP/3-21G calculations, N3 atom indicated the greatest values of proton affinity which means that N3 is more basicity than N2.

A few studies have been achieved to study the coordination chemistry of 1,2,3-selenadiazole ligands [29]. These studies indicated that the coordination between metal and 1,2,3-selenadiazole ring might be through N2 in 4-methyl-1,2,3-selenadiazole [30-32] or through N3 in 4-(2-pyridyl)-1,2,3-selenadiazole [33]. Connecting this N3 atom into coordination becomes more likely because of the metal chelation with the pyridinyl nitrogen and the nearby selenadiazole-N3.

In an attempt to detect the donor atom on 1,2,3-selenadiazole ring which is coordinating with $[VO(acac)_2]$, various 4-(*para*-substituted phenyl)1,2,3-selenadiazole molecules have been selected to be bound with vanadium atom in $[VO(acac)_2]$ through Se, N2 and N3. The resulting molecules have been selected to adopt *cis* or *trans* isomer.

Scheme 2 denotes the structures formula of *cis* and *trans* $[VO(acac)_2L]$ adducts. The donor atom (Se, N2 and N3) of 4-(*para*-substituted phenyl)-1,2,3-selenadiazole may be coordinate *cis* or *tans* to the O-oxido. The studied molecules have been optimized by performing the molecular mechanics force field, where the lowest energy conformations are obtained.



L= *para*-Substituted phenyl -1,2,3-Selenadiazole

Scheme 2. Structures formula of *cis* and *trans* [VO(acac)$_2$**L**] adducts, the donor atoms (Se, N2, N3) in 4-(*para*-substituted phenyl)-1,2,3-Selenadiazole may coordinate ***cis*** or ***tans*** to the O-oxido.

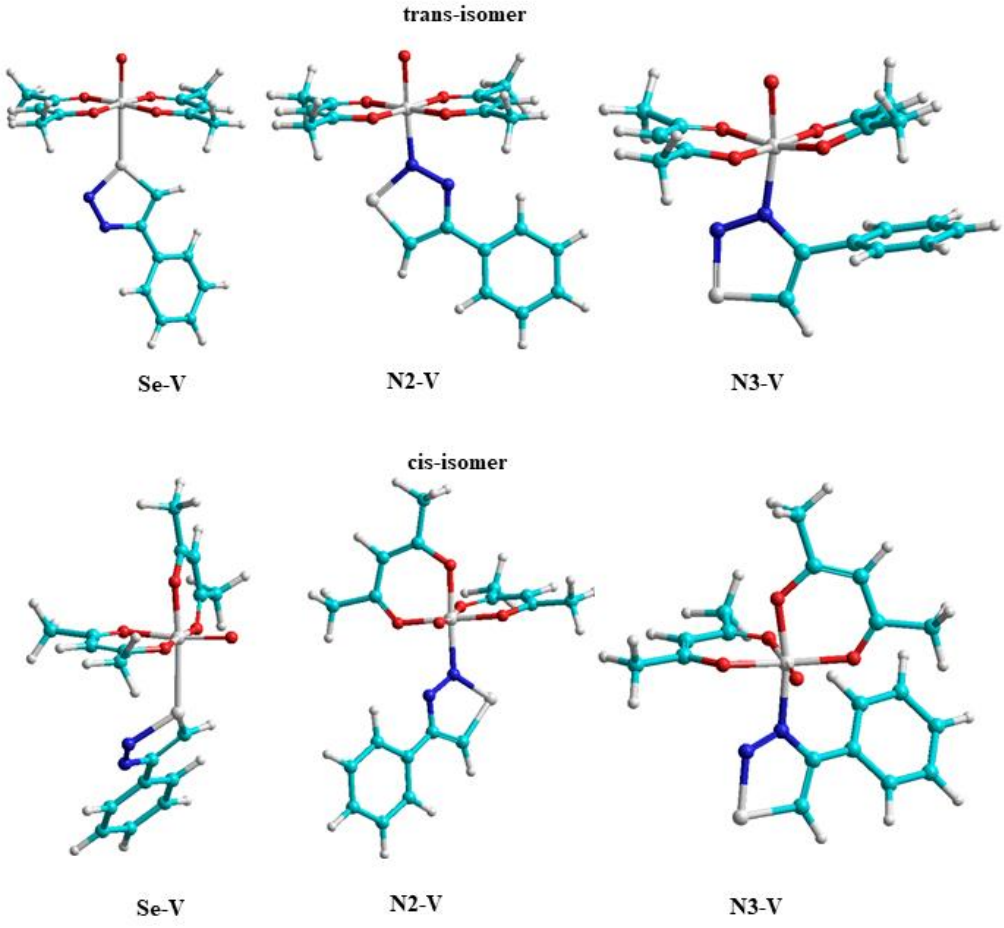


Figure1.Optimized structures formula of ***cis*** and ***trans***-[VO(acac)$_2$L] adducts isomers, the donor atoms (Se, N2, N3) in 4-(*para*-substituted phenyl)-1,2,3-selenadiazole may coordinate *cis* or *tans* to the O-oxido.

Figure 1 presents the optimized structures formula of *cis* and *trans* [VO(acac)$_2$L] adduct. L is 4-phenyl-1,2,3-selenadiazole.

Table 2. Total energy of conformations (in kcal/mol) of *cis* and *trans* [VO(acac)$_2$**L**] adducts, the donor atom (Se, N2 or N3) of 4-(*para*-substituted phenyl)-1,2,3-selenadiazole may coordinate *cis* or *tans* to the O-oxido.

X	***trans*-isomer**			***cis*-isomer**		
	Se-V	N2-V	N3-V	Se-V	N2-V	N3-V
H	50.377	47.993	50.862	51.046	23.988	39.657
CH_3	52.283	49.719	52.020	50.777	22.3659	39.122
Ph	60.881	58.343	60.010	49.901	23.306	37,867
NH_2	51.365	48.871	50.953	55.923	28.912	45.028
OCH_3	52.640	50.188	52.170	55.062	28.398	43.160
F	50.286	47.791	49.988	50.988	23.978	39.934
Cl	50.257	47.784	50.139	51.379	24.363	40.198
Br	50.050	47.549	49.512	51.512	24.480	40.237
CF_3	52.701	50.153	52.338	55.711	28.618	43.479
CN	53.185	49.524	51.415	51.566	24.286	39.468

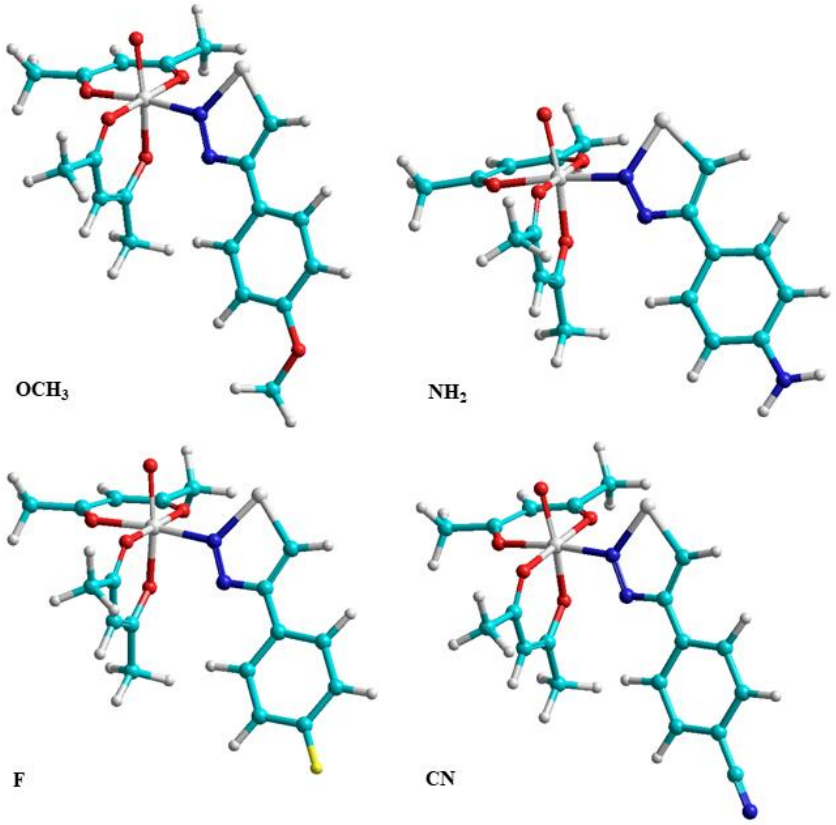


Figure 2. Optimized structures formula of ***cis***-[VO(acac)$_2$L] adduct. L is 4-(*para*-substituted phenyl)-1,2,3-selenadiazole.

Table 2 listed the total energy of *cis* and *trans* [VO(acac)$_2$**L**] adducts conformations. The results of the computed adducts revealed that all isomers of *cis* and *trans* adopted distorted octahedral. It can be

seen clearly form Table 2 that the *cis*-adduct isomers have the lowest total energy in comparison with *trans*-adduct isomers. It's means that these molecules may be more stable compared with other studied molecules. Furthermore, the *cis*-adducts isomers with N2-V binding have the lowest energy in comparison with the other *cis*-adducts isomer with Se-V or N3-V binding. Thus, the coordination of [$VO(acac)_2$] with 4-(*para*-substituted phenyl)1,2,3-selenadiazole molecules is more likely to be through N2 atom on the selenadiazole ring.

Table 3. Selected geometrical parameters of *cis*-[$VO(acac)_2$**L**] adducts, L is 4-(*para*-substituted phenyl)-1,2,3-selenadiazole calculated using BLYP/3-21G calculation. N2 atom is coordinated *cis* to the O-oxido.

X	H	CH_3	Ph	NH_2	OCH_3	F	Cl	Br	CF_3	CN
Bond distance (Å)										
V=O (oxo)	1.789	1.789	1.789	1.789	1.789	1.789	1.789	1.789	1.789	1.789
V-O [a] (ketonic)	1.854	1.854	1.854	1.855	1.854	1.854	1.854	1.855	1.854	1.854
V-O [b] (enolic)	1.850	1.850	1. 854	1. 850	1. 851	1. 850	1. 850	1.850	1. 854	1. 850
V-N2	1.917	1.917	1.920	1.917	1.917	1.917	1.917	1.918	1.919	1.917
Se-N2	1.834	1.834	1.835	1.833	1.834	1.834	1.833	1.834	1.834	1.834
N2=N3	1.252	1.253	1.253	1.252	1.252	1.252	1.252	1.252	1.253	1.252
N3-C4	1.267	1.267	1.267	1.267	1.267	1.267	1.267	1.267	1.267	1.267
C4=C5	1.342	1.342	1.342	1.342	1.342	1.342	1.342	1.342	1.342	1.342
C5-Se	1.879	1.879	1.879	1.880	1.879	1.880	1.880	1.879	1.879	1.879
Bond angle (°)										
O=V-O	170.08	169.85	177.90	170.00	169.95	170.28	170.19	170.83	176.09	169.72
O-V-O	96.09	96.09	80.23	95.97	96.03	95.98	95.91	95.81	95.78	90.03
O=V-N2	98.20	98.28	91.25	98.26	98.46	98.10	98.16	91.27	90.69	98.34
V-N2-Se	121.85	121.71	122.43	121.89	121.89	121.86	121.88	122.35	122.53	121.89
V-N2=N3	120.12	120.25	119.98	120.10	120.08	120.13	120.10	119.76	119.77	120.07
Se-N2=N3	118.03	118.04	117.59	118.01	118.04	120.13	118.01	117.89	117.71	118.03
N2-Se-C5	78.88	78.89	79.13	78.88	78.89	78.89	78.87	78.96	70.07	78.89
Se-C5=C4	113.34	113.34	113.19	113.36	113.31	113.34	113.37	113.32	113.23	113.32
C5=C4-N3	113.95	113.97	113.96	113.91	114.00	113.94	113.91	113.93	113.96	113.98
Bond dihedral (°)										
N3-C4´-C1´-C2´	-0.17	-0.36	0.10	-0.16	0.15	-0.09	-0.10	-0.07	0.48	-0.30
C5-C4-C1´-C6´	-0.13	-0.21	0.00	-0.05	0.00	-0,09	-0.05	0.03	-0.23	-0.21

Further geometry optimization has been carried out for the *cis*-[$VO(acac)_2$L] adducts at the B3LYP/STOG and B3LYP/3-21G levels of theory in order to study the structural and electronic properties of resulting adducts. Figure 2 presents the optimized structures formula of *cis*-[$VO(acac)_2$L] adduct. Table 3 shows the selected geometrical parameters of *cis*-[$VO(acac)_2$L] adducts, calculated using BLYP/3-21G method. The experimental data of crystallography of [$VO(acac)_2$] and 4-(4-Chlorophenyl)-1,2,3-selenadiazole moieties have reported [34,35]. It is very useful to compare these data with the theoretical data that calculated by B3LYP/3-21G method.

The optimized structures of the studied molecules indicate to have a distorted octahedral geometry. The bonds angle of O=V-O and O-V-O gave values in the range of 169.72-177.9 and 80.23-96.09

respectively. As shown in Table 3, the length of V=O (oxo) bond was 1.789 Å compared with 1.586 Å in free [$VO(acac)_2$] [25]. The calculated bond length of V-O (ketonic) and V-O (enolic) bonds in the adducts vary from 1.850 to 1.855 Å compared with 1.973 Å and 1.967 Å respectively in the free [$VO(acac)_2$]. Concerning 1,2,3- selenadiazole ring, the experimental bonds length of Se-N2, N2=N3, N3-C4, C4=C5 and C5-Se were 1.857, 1.265, 1.381 and 1.353 Å respectively in 4-(4-Chlorophenyl)-1,2,3-selenadiazole [26]. On the other hand, the experimental bonds angle of Se-N2=N3, N2-Se-C5, Se-C5=C4 and C5=C4-N3 were 111, 86.42, 111.9, and 113.1 (°) respectively in 4-(4-Chlorophenyl)-1,2,3-selenadiazole [26]. All these values are in good agreement with the calculated values, see Table 3. Finally, there is no clear trend for the variation of electronic donating or withdrawing groups on the structural properties of the studied adducts.

Some of the calculated energies of *cis*-[$VO(acac)_2L$] adducts using BLYP/STOG and BLYP/3-21G calculations are given in Table 4. The Binding energy of adducts formation and the reorganization energy of 4-(*para*-substituted phenyl)-1,2,3-Selenadiazole and [$vo(acac)_2$] in the adducts using BLYP/3-21G calculation are given in Table 5.

Table 4. Some of the calculated energies of *cis*-[$VO(acac)_2$**L**] adducts, L is 4-(*para*-substituted phenyl)-1,2,3-selenadiazole calculated using BLYP/STOG and BLYP/3-21G calculations. N2 atom is coordinated *cis* to the O-oxido.

X	**Methods**	**Binding energy kcal/mol**	**E_{HOMO} eV**	**E_{LUMO} eV**
H	STOG	-2736528.57	-5.661	-3.884
	3-21G	-2506056.73	-9.762	-7.882
CH_3	STOG	-2760219.78	-5.444	-3.642
	3-21G	-2061255.01	-9.545	-7.578
Ph	STOG	-2372471.90	-5.345	-3.467
	3-21G	-2484322.38	-9.657	-7.802
NH_2	STOG	-2769768.20	-5.469	-3.6
	3-21G	-2098283.03	-9.834	-7.732
OCH_3	STOG	-2777009.67	-5.499	-3.622
	3-21G	-2151226.07	-9.945	-7.711
F	STOG	-2796070.93	-5.696	-3.679
	3-21G	-2148539.39	-9.563	-7.43
Cl	STOG	-2976746.76	-5.36	-3.34
	3-21G	-2244784.61	-9.472	-7.23
Br	STOG	-4295115.76	-5.803	-3.742
	3-21G	-4105436.87	-9.603	-7.216
CF_3	STOG	-2616844.67	-5.106	-3.121
	3-21G	-1971597.43	-9.754	-7.301
CN	STOG	-2515070.12	-5.14	-3.162
	3-21G	-1957462.17	-9.876	-7.233

The binding energy of adduct formation reactions has been calculated by the difference between the binding energy of *cis*-[$VO(acac)_2L$] adduct and that of individual [$VO(acac)_2$] and 4-(*para*-substituted phenyl)-1,2,3-selenadiazole ligand. Also, the reorganization energy of ligands and [$VO(acac)_2$] that is needed to change the geometry of them into that present in the final [$VO(acac)_2L$] adduct has been calculated [36-37].

As shown in Table 5, the values of binding energy are somewhat large values (vary from 1066083.30 to 321355.55 kcal/mol) these may be due to needing to overcome steric interactions of $[VO(acac)_2]$ and 4-(*para*-substituted phenyl)-1,2,3-selenadiazole ligands.

The organization energy of $[VO(acac)_2]$ represents the required energy to convert the geometry of vanadyl complex from a square pyramidal to distorted octahedral, while the organization energy of ligands represents the required energy to change the bonds lengths and angles of free ligand into that present in adduct. It can be seen clearly form Table 5 that the required energy to convert the geometry of vanadyl complex from a square pyramidal to distorted octahedral is almost similar (vary from 29.94-30.66 kcal/mol). On the other hand, the organization energy of ligand was different values for each ligand (vary form 20.44-23.90 kcal/mol).

Figure 3 shows the spatial distribution of the highest molecular orbital (HOMO) and lowest unoccupied molecular orbital of selected adducts. The negative region is showed with violet color, while the positive region is showed with green color. In general, HOMOs orbitals are located mainly on the nitrogen atom in diazole ring and on $[VO(acac)_2]$ moiety. In contrast, LUMOs orbitals are located mainly on$[VO(acac)_2]$ moiety and on different atoms (Se, N and C) in selenadiazole moiety. In other words, from the diagrams of HOMO and LUMO, it can be concluding existence two types of interaction between nitrogen and vanadium atoms in the adducts. First type of interaction is pπ-dπ, where the nitrogen atom donates pairs of electrons to vanadium atom to form σ covalent bond. The second type of interaction is dπ-pπ, where the vanadium atom donates single electron to nitrogen atom to form π bond. These two types of interactions are illustrated in Figure 4.

Table 5. The Binding energy of adducts formation and the reorganization energy of 4-(*para*-substituted phenyl)-1,2,3-Selenadiazole and $[vo(acac)_2]$ in the adducts using BLYP/3-21G calculation.

X	ΔE [a] kcal/mol	E_{reorg} of L [b] kcal/mol	E_{reorg} of $[vo(acac)_2]$ [c] kcal/mol
H	321355.55	23.50	30.14
CH_3	790676.75	23.17	30.45
Ph	487183.07	20.89	29.94
NH_2	763650.40	22.36	30.05
OCH_3	747617.61	23.72	30.43
F	740787.81	23.90	30.55
Cl	869602.35	20.44	30.12
Br	329069.26	21.23	30.66
CF_3	1066083.36	20.69	30.01
CN	927484.28	29.85	30.00

[a] The binding energy of adduct formation which is calculated by the difference between the energy of the adduct and that of the individual 4-(*para*-Substituted phenyl)-1,2,3-selenadiazole and $[vo(acac)_2]$ moieties.
[b] Reorganization energy of 4-(*para*-substituted phenyl)-1,2,3-selenadiazole. [c] Reorganization energy of $[vo(acac)_2]$.

4. Conclusions

In the present investigation we have investigated the adducts formed between $[Vo(acac)_2]$ and 4-(*para*-substituted phenyl)-1,2,3-selenadiazole ligands.
The studied ligands have more than one donor atoms (Se, N2 and N3) that may coordinate with

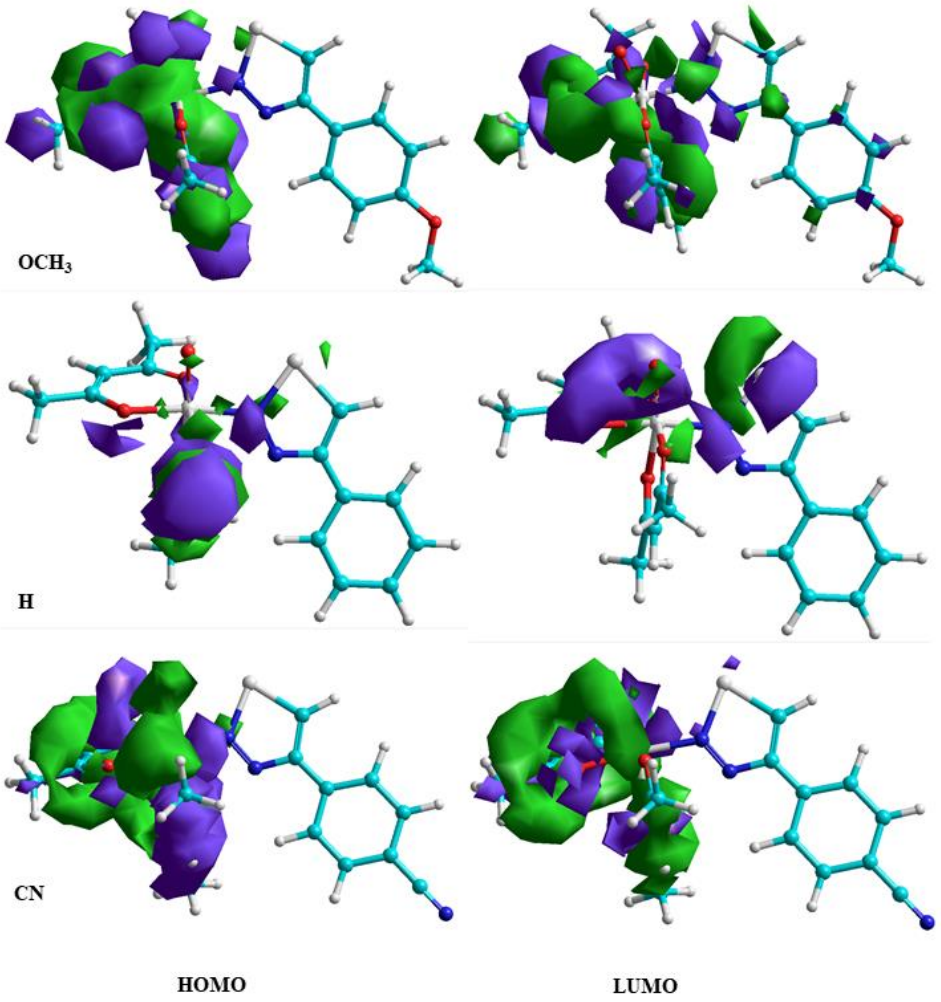


Figure 3. Molecular orbital spatial distribution for the HOMO and LUMO of ***cis***-[VO(acac)$_2$L] adduct. L is 4-(*para*-substituted phenyl)-1,2,3-Selenadiazole.

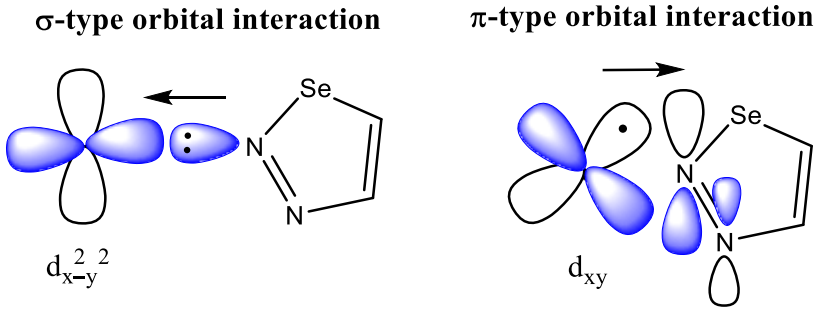


Figure 4: interaction types of selenadiazole ring with d orbitals of vanadium atom

vanadium atom on the [Vo(acac)$_2$]. In an attempt to detect the donor atom on 1,2,3-selenadiazole ring which is coordinating with [VO(acac)$_2$], the 4-(*para*-substituted phenyl)1,2,3-selenadiazole molecules have been selected to be bound with vanadium atom in [VO(acac)$_2$] through Se, N2 and N3. The resulting adducts have been investigated in two geometries (*cis* and *trans*) in order to show the effect of such structural change on the electronic properties of the studied adducts. Based on the electron

density of nitrogen atoms, calculations of basicity of nitrogen atom and calculations of lowest energy conformation, the suggested structures of adducts of [$VO(acac)_2$] with 4-(*para*-substituted phenyl)1,2,3-selenadiazole molecules have been detected.

The resulting structure of adduct have been studied at two levels of DFT theory to investigated their structural and electronic properties. The structural properties (i.e. bond lengths and angles) of the studied [VO(acac)2] and 4-(*para*-substituted phenyl)1,2,3-selenadiazole moieties indicated a good agreement with experimental data of free molecules.

The organization energy of both [$VO(acac)_2$] and 4-(*para*-substituted phenyl)1,2,3-selenadiazole moieties into that present in adducts have been calculated, where the required energy to convert the geometry of vanadyl complex from a square pyramidal to distorted octahedral was almost 30 kcal/mol. The HOM and LUMO spatial distribution indicated interesting interactions between nitrogen and vanadium atoms.

The variation of electronic donating or withdrawing groups on the structural properties of the studied adducts have no interesting effects on the structural and electronic properties of the studied adducts. Finally, the new adducts species have interesting properties and deserve to be investigated experimentally.

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