The Effect of Substituents on Catalytic Performance of *bis*-Thiosemicarbazone Mo(VI) Complexes: Synthesis and Spectroscopic, Electrochemical, and Functional Properties¹

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Abstract—The preparation, characterization and electrochemical properties are reported for three new types of molybdenum(VI) complexes with *bis*-thiosemicarbazone ligands. All compounds were characterized by elemental analysis, electronic spectra, IR and ¹H NMR spectroscopies, thermogravimetric analysis, and cyclic voltammetry. The *bis*-thiosemicarbazone Mo(VI) complexes were tested as a catalyst for the homogeneous oxidation of olefins using *tert*-butyl hydrogen peroxide as an oxidant. The catalysts showed efficient reactivity in the olefins epoxidation reactions giving high yield and selectivity of the products, in most cases. Results showed that the *bis*-thiosemicarbazone ligands introduced both electronic and steric effects on catalytic performance of the prepared Mo(VI) complexes.

Keywords: dioxomolybdenum(VI) complex, *bis*-thiosemicarbazone, olefin epoxidation **DOI:** 10.1134/S002315841802012X

Thiosemicarbazone derivatives represent important class of Schiff base ligands with wide pharmacological versatility [1-3]. The chemistry of thiosemicarbazones, mixed hard-soft nitrogen-sulfur chelating ligands, bounded to metals have also attracted considerable interest primarily due to their medicinal properties including antibacterial, antitumour, antiviral and antifungal properties [4-7]. Some experimental evidences supported the relationship between chemical structures and biological activities of α -(N)-heterocyclic thiosemicarbazones and their metal complexes [8]. Experimental results showed that the changes in the ligand backbone can significantly alter the biological activity of the thiosemicarbazones [9]. *bis*-Thiosemicarbazones are subgroups of thiosemicarbazones which have exhibited very interesting pharmacological properties [10, 11]. They were also investigated as potential nuclide carriers for medical imaging [12]. Due to their higher denticity, bisthiosemicarbazones have ability to link metal ions more strongly than thiosemicarbazones [13]. Because of important chemical properties and potentially biological activities of both the ligands and the complexes, the investigation of more effective thiosemicarbazone metal complexes is constantly progressing.

Synthesis and characterization of molybdenum compounds with sulfur donor atoms has been drawing considerable attention ever since their relevance to the active sites of different oxotransfer enzymes was discovered [14–16]. The extended X-ray absorption fine structure (EXAFS) spectroscopic studies on active sites of molybdoenzymes such as sulfite oxidase, nitrate reductase, and xanthine dehydrogenase have shown that the coordination environment of Mo in both oxidized and reduced forms, i.e. Mo^{V1}O₂ and Mo^{IV}O₂ units, involves at least two sulfur atoms in form of thiolate rather than thioether ligands [17]. Apart from the biological significance, higher valent Mo complexes are also well known for their useful application in industrial redox processes such as epoxidation of olefins, olefin metathesis and isomerization of allylic alcohols [18, 19].

Recently, we have described the synthesis of dioxomolybdenum(VI) complex with the formula $[MoO_2L(CH_3CN)]$ (L = 1-(2,4-dihydroxybenzylidene)-N-methyl-N-phenylthiosemicarbazone) which exhibited high catalytic activity for epoxidation of olefins [20]. In this study, the synthesis, characteristics, and catalytic performance of three new molybdenum(VI) complexes with *bis*-thiosemicarbazone ligands have been described. We have aimed to study the effect of ligand substituents on the spectroscopic, electrochemical, and functional properties of Mo(VI)

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complexes. The catalytic properties of the reported complexes are also described for the homogeneous epoxidation of olefins using *tert*-butyl hydrogen per-oxide (TBHP) as an oxidant.

EXPERIMENTAL

Materials

Commercial reagents hydrazine hydrate (Merck) and 2,6-diacetylpyridine (Aldrich), N-methyl aniline (Merck), carbone disulfide (Merck) were used as received. 4-Methyl-4-phenyl-3-thiosemicarbazide [21], 4-phenyl-3-thiocabazide and *p*-chlorophenylth-iosemicarbazide [22] were prepared according to literature procedures. The starting complex, *bis*-(acetylacetato) dioxomolybdenum(VI) [MoO₂(acac)₂] was prepared as described in the report [23].

Instrumentation and Physical Measurements

Elemental analysis (C, H, N) data were performed on a Perkin Elmer 2400 CHNS/O elemental analyzer. IR measurements of the solids were carried out on a Unicam Matson 1000 FT-IR spectrophotometer (400–4000 cm⁻¹). NMR spectra were obtained on a Bruker 500-DRX Avance Spectrometer in DMSO-d₆.UV-vis spectra were recorded by CARY 100 Bio VARIAN UV-vis spectrophotometer using quartz cells having a 1.0 cm path in length. Melting points of the products were monitored on a BUCHI Melting Point Modle B-540. Thermogravimetric (TG) analyses were measured on a NETZSCH TG 209 F1 Iris thermobalance using aluminum crucibles under nitrogen atmosphere with a heating rate of 10°C/min. For all experiments, the temperature ranged from 20 to 900°C. The cyclic voltammetric measurements were made on a Autolab/PGSTAT101 electrochemical analyzer utilizing the three-electrode configuration of a Ag/AgCl as reference electrode, a Pt auxiliary electrode, and Pt working electrode. NOVA software was employed to carry out the experiments and to acquire the data. The working electrode was polished fresh before each experiment with alumina and sonicated in deionised water. The tests were performed in the potential region -0.8 to +1 V at ambient temperature at a scan rate of 20 mV/s. Recrystallized tetra(*n*-butyl)ammonium perchlorate (**TBAP**) (0.01 mol/dm³) was used as supporting electrolyte and DMF as solvent.

Preparation of the Ligands

All Schiff base ligands L^1 , L^2 and L^3 were synthesized in a similar way by the condensation reactions of 2,6-diacetylpyridine with corresponding thiosemicarbazide in a 1 : 2 ratio. A typical preparation of the ligands is described as follow.

2,6-Diacetylpyridine *bis*-(4-methyl-4-phenylthiosemicarbazone) (L¹). 0.180 g (1.1 mmol) of 2,6-diacetylpyridine in 10 mL methanol was added to 40 mL methanolic solution of 0.400 g (2.2 mmol) of 4-methyl-4-phenyl-3-thiosemicarbazide. The solution mixture was refluxed with vigorous stirring for 8 h and left for slow evaporation for the final separation of a solid compound. The bright yellow precipitate was filtered. The crude product was recrystallized from a methanol-ether mixture and dried in air. M.p.: 232°C, yield 0.296 g, 55%. For $C_{25}H_{27}N_7S_2$, %: calculated: C 61.32, H 5.56, N 20.02; found: C 61.95, H5.67, N 20.39.

Similar procedures were applicable to the preparations of L^2 and L^3 .

2,6-Diacetylpyridine *bis*-(4-phenylthiosemicarbazone) (L²). M.p: 222°C, yield 0.330 g, 65%. For $C_{23}H_{23}N_7S_2$, %: calculated – C 59.84, H 5.02, N 21.24; found – C 59.34, H 4.45, N 20.66.

2,6-Diacetylpyridine *bis*-(4-parachlorophenylthiosemicarbazone) (L³). M.p: 215°C, yield 0.397 g, 68%. For $C_{23}H_{21}N_7S_2Cl_2$, %: calculated – C 52.07, H 3.99, N 18.48; found – C 52.82, H 4.34, N 18.26.

Preparation of the Complexes

Complexes $[MoO_2L^1]$ (1), $[MoO_2L^2]$ (2) and $[MoO_2L^3]$ (3) were prepared in a similar way by refluxing methanolic solutions of $MoO_2(acac)_2$ (0.6 mmol, 0.200 g) with H_2L^1 (0.6 mmol, 0.294 g), H_2L^2 (0.6 mmol, 0.277 g) and H_2L^3 (0.6 mmol, 0.318 g), respectively. Initially on mixing, the solutions turn to brown color and after refluxing for 4 h, the dark brown complexes separated. The mother liquors were cooled and left for slow evaporation for the final separation of solid compounds. The solids were washed with methanol and diethyl ether and dried under vacuum. Our attempts to get single crystals suitable for X-ray diffraction studies were not successful. Scheme 1 illustrates the syntheses of complexes.

 $[MoO_2L^1] \cdot H_2O$ (1): yield 0.220 g, 55%. For $C_{25}H_{27}N_7S_2MoO_3$, %: calculated: C 47.39, H 4.29, N 15.47; found: C 47.18, H 3.96, N 16.50.

 $[MoO_2L^2] \cdot H_2O$ (2): yield 0.100 g, 55%. For $C_{23}H_{23}N_7S_2MoO_3$, %: calculated: C 45.62, H 3.83, N 16.19; found: C 45.22, H 3.67, N 16.34.

 $[MoO_2L^3]$ (3): yield 0.150 g, 55%. For $C_{23}H_{19}N_7S_2$ -Cl₂MoO₂, %: calculated: C 42.08, H 2.92, N 14.94; found: C 42.62, H 2.66, N 14.86.

Schematic representation of *bis*-thiosemicarbazone ligands and complexes 1-3

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Catalytic Reactions

1 mmol of TBHP (oxidant) was added to a solution of alkene (1 mmol), $[MoO_2L^1]$ (0.001 mmol) and chlorobenzene (1 mmol), as internal standard in appropriate solvent (1 mL). The system was stirred for 1–5 h at 75°C. The progress of the reaction was monitored by GC. All the reactions were performed at least two times and the products were compared with standard samples.

RESULTS AND DISCUSSION

Synthesis of bis-Thiosemicarbazone Mo(VI) Complexes

The dioxomolybdenum(VI) complexes were synthesized by the reaction of *bis*-(acetylacetonato)dioxomolybdenum(VI) with a stoichiometric amount of *bis*-thiosemicarbazone ligands derived from 2,6-diacetylpyridine and corresponding N4-substituted thiosemicarbazide, in methanol solution. These dark brown complexes were found to be sparingly soluble in alcohol, CHCl₃, and CH₂Cl₂, but fairly soluble in DMF and DMSO. In the investigated monomeric [MoO₂L] complexes, each of the Schiff base ligands behaves in a dianionic tetradentate manner, bonded to the *cis*-MoO₂²⁺ ion through the sulfur and azomethine nitrogen atoms. The formulations are in accordance with the data of elemental analysis and physicochemical measurements.

FT-IR Spectra

Table 1 lists the tentative assignments of the main IR bands of the dioxomolybdenum(VI) complexes for the ligands H_2L^1 , H_2L^2 and H_2L^3 in 4000–400 cm⁻¹ region. The free ligands show medium-intensity bands at 3230 cm⁻¹ assigned to NH vibrations of the functional group, which disappear in the corresponding complexes, indicating possible deprotonation of the functional group upon complexation [24, 25]. This evidence is further confirmed by NMR spectra. A

strong band due to v(C=N) appears at 1600 cm⁻¹ in the free ligands, and this band undergoes a bathochromic shift by $4-10 \text{ cm}^{-1}$ in the complexes, thereby indicating the participation of azomethine nitrogens in coordination. Characteristic strong bands in the spectra of H_2L^2 and H_2L^3 observed in the region 3420-3340 cm⁻¹ attributed to modes of the NH group which remain at nearly the same position in the spectra of the corresponding complexes, suggesting the non-involvement of this amino group in bonding [26]. The v(N-N)of the thiosemicarbazone is found at ~ 1119 cm⁻¹. The increase in the frequency of this band in the spectra of the complexes, due to an increase in the bond strength, again confirms coordination via the azomethine nitrogen [27]. The decrease in the stretching frequency of the v(C=S) band from ~816 cm⁻¹ in the thiosemicarbazones by $60-75 \text{ cm}^{-1}$ upon complexation indicates coordination via the thiolato sulfur, a commonly observed feature of such ligands [28]. IR spectra of complexes 1-3 show sharp bands at ~1540 cm⁻¹ due to the newly formed v(N=C) bond, indicating the coordination of sulfur in the enolate form rather than in the keto form [29, 30]. All monomeric neutral complexes 1-3 exhibit two bands at ~903-910 and 935-951 cm^{-1} assigned to symmetric and antisymmetric vibrations of the cis-dioxomolybdenum(VI) moiety, respectively [31]. IR spectra of compounds $[MoO_2L^1]$ and $[MoO_2L^2]$ show broad bands around 3430 cm⁻¹ which indicate the presence of lattice water.

NMR Spectra

¹H NMR spectra of H_2L^1 , H_2L^2 and H_2L^3 and their molybdenum complexes were recorded in DMSO-d₆ solvent and data with their assignments are listed in Table 2. The ¹H NMR spectra of all ligands exhibit similar signals (δ , ppm) at (10.96, 2.42), (10.86, 2.64) and (10.80, 2.54) which can be assigned to 2(NH^a) and 2(CH₃^c) protons, respectively. The signals correspond-

Compound	ν(N–H)	v(C=N)	ν(N=C)	ν(N–N)	v(C=S)	v(Mo=O)	
						(sym)	(asym)
H_2L^1	3222	1592	-	1113	819	—	—
$[MoO_2L^1]$	—	1596	1544	1155	758	951	910
H_2L^2	3232, 3422	1602	—	1129	816	-	—
$[MoO_2L^2]$	3418	1598	1551	1161	752	951	903
H_2L^3	3235, 3457		—	1116	816	-	—
[MoO ₂ L ³]	3396	1592	1515	1158	749	935	910

Table 1. Wavenumbers (cm^{-1}) of the characteristic IR bands of the ligands and corresponding dioxomolybdenum(VI) complexes

Table 2. ¹H NMR spectra of H_2L^1 , H_2L^2 and H_2L^3 ligands and their molybdenum complexes recorded in DMSO-d₆ as solvent

Assignment	δ, ppm			δ, ppm			
	H_2L^1	H_2L^2	H_2L^3	$[MoO_2L^1]$	$[MoO_2L^2]$	$[MoO_2L^3]$	
H ^a (s, 2NH)	10.96	10.86	10.80	_	_	_	
H ^b (s, 2NH)	—	10.45	10.24	—	9.85	10.25	
H ^c (s, 2CH ₃)	2.42	2.64	2.54	3.17	3.17	3.18	
H ^d (s, 2CH ₃)	3.58	_	_	3.39	_	_	
H ^e (d, 2CH)	8.37	8.31	8.57	8.03	8.17	8.35	
H ^f (t, 2CH)	7.93	7.89	7.86	7.71	7.85	7.89	

ing to NH^b in H_2L^2 and H_2L^3 and also the signal of CH₃^d in H I¹ are observed at 10.51 10.24 and 3.58 ppm

in H_2L^1 are observed at 10.51, 10.24 and 3.58 ppm, respectively. These observations prove the thione form of the ligand in solution. Peaks of the aromatic protons of the phenyl groups were found in the region 7-7.6 ppm. A triplet signal at 7.93, 7.89, and 7.86 ppm and a doublet at 8.37, 8.31, and 8.56 ppm for H_2L^1 , H_2L^2 and H_2L^3 , respectively, correspond to the protons of the pyridine moiety. In NMR spectra of the complexes, the signals due pyridine moiety and NH^b (in complexes $[MoO_2L^1]$ and $[MoO_2L^2]$) appeared mostly at the same position as in the free ligands, indicating the non-involvement of pyridine nitrogen and NH^b in coordination. The coordination of the C-S groups in complexes is supported by absence of NH^a proton signals in the spectra of the three complexes that is in accordance with the formulation of thioenolization and subsequent the replacement of the protons by metal [32]. Signals due to CH₃^c protons show a remarkable shift in complexes 1-3, suggesting the involvement of the azomethine nitrogen in coordination to metal ions.

Electronic Spectra

Electronic absorption bands of the ligands and complexes were studied in a DMF solution. The compounds are found to display similar absorption maxima in the range 200–350 nm which assigned to intraligand transitions (Fig. 1). The complexes 1–3 exhibit one low-energy electronic absorption band in the region 400–500 nm which may be assigned to a charge-transfer transition from $p\pi$ -orbital of sulfur (HOMO) to the $d\pi$ -orbital of molybdenum (LUMO) [20, 33]. The absence of a d-d-transition absorption band in the visible region confirms the $4d^0$ electronic configuration of Mo(VI). Complexes 1–3 show similar electronic spectra, suggesting that they have essentially similar structure.

Electrochemical Studies

Cyclic voltammograms of the ligands (H_2L^1, H_2L^2) and H_2L^3) and their dioxomolybdenum(VI) complexes **1–3** were recorded at a platinum electrode using DMF as solvent and tetrabutylammonium perchlorate (TBAP) as supporting electrolyte at a scan rate of 20 mV/s in the potential range +1 to -0.7 V vs. Ag/AgCl reference. Ligands, L¹, L² and L³ exhibited one irreversible oxidative peak around 0.3 V. Complexes 1-3 exhibited irreversible single-electron reduction waves in their cyclic voltammograms attributable to a reduction at the molybdenum centers (Fig. 2). Previously, it has been shown that the substituent on the ligand has a significant effect on the cathodic reduction potential [34, 35]. The effect of these groups, although not intimately linked to the molvbdenum, is to alter the electron density on the metal center. The more negative is the cathodic reduction potential, the more difficult is the molybdenum complex reduction [36]. The electron donating group, CH_3 on azomethine carbon in L^1 is probably the leading contributor to increasing electron density at the Mo(VI) center in $[MoO_2L^1]$. In this case, the cathodic reduction potential is the most negative of the series. Again, since the Cl substitution at position 5 of the phenyl ring in L^3 is electron withdrawing, it is expected that the electron density is shifted away from Mo(VI) center, the complex [MoO₂L³] becomes easily reducible and the cathodic peak potential (E_{pc}) shifts towards the anodic direction, compared to $[MoO_2L^2]$. This type of behavior was also noted earlier for other dioxomolybdenum(VI) complexes [35].

Thermal Properties

The thermogravimetric analysis of the complexes was carried out in the temperature range 20-900°C at a heating rate of 10°C/min (Fig. 3). Complexes $[MoO_2L^1]$ and $[MoO_2L^2]$ showed weight losses in the temperature range 80–110°C that could be due to the removal of lattice water molecule. In complex 3, there was no weight loss in the region below 200°C which showed the absence of water molecule. With further elevation in temperature, the TG curves showed two steps of weight losses. The first step of decomposition observed in the range from 200 to 400°C may be ascribed to the dissociation of the Schiff base ligand at the C=N bond. The last stage at $630-720^{\circ}$ C can be ascribed to the complete removal of the fragment parts of the ligand. Decomposition continued until the final residue MoO₃ was left [37].

Epoxidation of Olefins

The catalytic performance of $[MoO_2L^1] \cdot H_2O$ was first studied in the oxidation of cyclooctene, used as a model substrate, with TBHP as the oxygen donor and the results are shown in Table 3. The effect of various reaction media on the oxidation of cycloctene has been studied. It is apparent that the efficiency of the catalyst in different solvents decreases in the order: dichloroethane>dichloromethane > acetonitrile > methanol > DMF. Apparently, highly coordinating solvents such as CH₃OH and DMF cause a significant decrease in the catalytic activity, since they compete with TBHP to bind to the molybdenum center [38].

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Fig. 1. UV-vis spectroscopy of H_2L^1 , H_2L^2 and H_2L^3 ligands and their molybdenum complexes 1–3.



Fig. 2. Cyclic voltammogram of complexes $[MoO_2L^1](I)$, $[MoO_2L^2](2)$, and $[MoO_2L^3](3)$ in DMF (0.01 M TBAP as supporting electrolyte, scan rate: 20 mV/s).



Fig. 3. Thermogravimetric analysis of the complexes 1–3.

Entry	Catalyst, mmol	Temperature, °C	Solvent	Conversion, %	Selectivity, %
1	0.005	75	CH ₃ CN	51	93
2	0.005	75	CH ₂ Cl ₂	72	95
3	0.005	75	CH ₃ OH	38	99
4	0.005	75	DMF	31	98
5	0.005	75	$C_2H_4Cl_2$	82	99
6	0.001	75	$C_2H_4Cl_2$	85	99
7	0.0005	75	$C_2H_4Cl_2$	66	99
8	0.01	75	$C_2H_4Cl_2$	75	99
9	0.005	65	$C_2H_4Cl_2$	73	99
10	0.005	55	$C_2H_4Cl_2$	62	99
11	0.005	40	$C_2H_4Cl_2$	46	99
12	0.005	room	$C_2H_4Cl_2$	19	99

Table 3. Conversion of cyclooctene using $[MoO_2L^1]$ as catalyst for 1 h of reaction time under different reaction conditions

The effect of the catalyst amount on the conversion and selectivity is illustrated in Table 3. Four different amounts of catalyst viz. 0.01, 0.005, 0.001, and 0.0005 mmol were considered while keeping a fixed amount of cyclooctene (1 mmol) and TBHP (1 mmol). The results show that the decrease in the catalyst amount from 0.005 to 0.001 mmol did not have a significant effect on the percent of conversion under reaction conditions of this study (Table 3, entries 5 and 6). However, further decrease in the catalyst amount to 0.0005 mmol caused the conversion of cyclooctene to reach 66%. With a further increase in the catalyst amount from 0.005 to 0.01 mmol, the con-

Table 4. Catalytic oxidation of various alkenes with TBHP by $[MoO_2L^1]$ complex*

Substrate	Conversion, %**	Selectivity to epoxide, %	Time, h	
	85	99	1	
	86	>99	5	
	71	38	4	
\frown	23	>99	4	
	26	>99	4	

* Reaction condition. The molar ratio for catalyst: alkene: TBHP was 1 : 1000 : 1000. The reactions were run at 75°C in 1 mL of 1,2-dichlroethane.

** GC conversion based on starting alkene.

version showed a small reduction from 82 to 75% (Table 3, entries 5 and 8). Effect of reaction temperature on cyclooctene oxidation was investigated. It was inferred that 75°C was the best suited temperature for the maximum oxidation of cyclooctene under the above reaction conditions. Thus, optimized operating reaction conditions for maximum oxidation of cyclooctene were: cycloctene (1 mmol), $[MoO_2L^1]$ (0.001 mmol), TBHP (1 mmol), dichlroetane (1 mL), and reaction temperature (75°C).

In order to verify the catalytic scope of the $[MoO_2L^1]$ catalyst, it has also been applied for epoxidation of a wide variety of alkenes (Table 4). Good results are found for cyclic alkenes such as cyclohexene and cyclooctene, whereas terminal linear alkenes give slightly lower yields. In the epoxidation reaction of cyclohexene, no allylic oxidation products were detected, thus catalytic reaction occurs via nonradical processes [39]. In case of styrene oxidation the highest selectivity has been achieved for benzaldehyde, and this is possibly due to the nucleophilic attack of the oxidant to styrene oxide following by decomposition of the peroxy-styrene intermediate [40].

The catalytic activities of the prepared catalysts were studied through the oxidation of olefins with TBHP in 1,2-dicholoroethane. As the results in Fig. 4 show, the catalytic performance of the complexes decreased in the following order: $MoO_2L^2 > MoO_2L^3 > MoO_2L^1$.

Based on Kühnet al. report [41], olefins are oxidized by TBHP in a catalytic cycle involving the nucleophilic attack of the olefin to the coordinated oxygen (*) in the heptacoordinated intermediate containing coordinated peroxide and a protonated oxo ligand. The epoxide product is obtained by transfer of the oxygen atom of the $-OOC(CH_3)_3$ ligand to the olefin



Fig. 4. Epoxidation of cyclooctene with TBHP using various catalysts (75°C for 60 min in 1 mL of 1,2-dichlroethane).

C=C double bond. Herein, the metal center acts as a Lewis acid by removing charge from the O–O bond, facilitating its dissociation, and activating the nearest oxygen atom (*) for insertion into the olefin double bond. At the final stage, the release of a *tert*-butanol molecule from metal center leads to the formation of complex (Scheme 2). As the presence of the electron-withdrawing substituents on ligand induces more positive charge on the coordinated oxygen (*), we

expected the efficiency of the catalysts to decrease in the order: $[MoO_2L^3] > [MoO_2L^2] > [MoO_2L^1]$, while in fact the order observed for epoxidation of cyclooctene is: $[MoO_2L^2] > [MoO_2L^3] > [MoO_2L^1]$. This observation can be due to both electronic and steric effects of ligand substituents.

Proposed mechanism for oxidation of alkene with $[MoO_2L^1]$ complex in the presence of TBHP



CONCLUSIONS

In this study, three new types of molybdenum(VI) complexes with thiosemicarbazone ligands containing

a tetradentate N_2S_2 donor set to the central metal atom have been described. All compounds were characterized by physicochemical and spectroscopic techniques

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including elemental analysis, electronic spectra, IR and ¹H NMR spectroscopies, thermogravimetric analysis, and cyclic voltammetry. The thiosemicarbazone Mo(VI) complexes were also tested as catalysts for the homogeneous oxidation of olefins. The catalysts showed efficient reactivity in the olefins epoxidation reactions with good yield and selectivity. In addition, results confirm that the variation of substituents on the ligand structures can influence the spectroscopic, electrochemical, and functional properties of the Mo(VI) complexes and the catalytic reaction rates can be controlled by both electronic and steric factors.

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