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8-Hydroxyquinoline Complexes of Silicon: Synthesis, Characterization and Reactivity

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ABSTRACT

*A series of complexes were formed starting from the reaction of 8-hydroxyquinoline with chlorotriethoxysilane and phenytrichlorosilane to give penta coordinate complexes, namely 8-(triethoxysilyloxy)quinoline (**1**) and 8-(dichloro(phenyl)silyloxy)quinoline (**2**) respectively. Complex (**1**) was reacted with tripodal ligands like 2,2′,2″-*nitrilotriacetic acid and *tris(2-hydroxy-3,5-dimethylbenzyl)amine* leading to the synthesis of silatranes (**3-4**). Further, the reactions *of complex (**2**) with potassium isothiocyanate, catechol and N-methyldiethanolamine yielded novel hypervalent complexes of silicon (**5-7**). All the complexes have been characterized by elemental analyses, infrared spectroscopy, ^{1}H, ^{13}C NMR spectroscopy and mass spectrometry. The spectral data showed that 8-hydroxyquinoline acted as a monobasic bidentate ligand with N,O-donor sites. The thermal stability of the complexes was studied by thermogravimetric analysis and the experimental results have been correlated with computational studies.*

Keywords: 8-hydroxyquinoline; chlorotriethoxysilane; phenytrichlorosilane; silatrane; hypervalent; thermogravimetric analysis.

INTRODUCTION

The assorted chemistry of hypervalent silicon compounds is varied in both structures and reactivity[1-4], and has generated a flurry of innovative research endeavors in recent years[5-9]. The number of hypervalent silicon compounds has grown remarkably, and they exhibit novel structural features, unusual chemical and biological activity and potential application in different fields such as organic synthesis, catalysis, medicines, material sciences and engineering[10-14].

The biologically active bidentate ligand 8-hydroxyquinoline has been widely used to study higher coordination in main group metal coordination chemistry[15-16]. 8-Hydroxyquinoline (8-HQ) and its derivatives are widely used as chelating reagents in analytical chemistry and radiochemistry for metal ion extraction and fluorimetric determination[17]. They can perform as structurally related subunits in important biomolecules or biochemical processes, which show strong cytotoxic and antimicrobial properties, and represent the main component in some bactericide, fungicide and antimalarial drugs[18-19]. In recent years, metal chelates of 8-HQ have played an important role in organic electroluminescence (OEL) and are widely introduced in OEL cell emission layer[20]. A few higher-coordinate silicon(IV)

complexes with 8-hydroxyquinoline type of ligand have been reported in the literature[21-24]. The X-ray structure analyses delivered the various insights into the great variability of coordination spheres of higher-coordinate silicon and tin with two chelating 8-oxyquinolinato moieties[25-27].

The present work describes the synthesis, characterization and reactivity of some novel hypervalent silicon(IV) complexes with the 8-hydroxyquinoline ligand coordinating via deprotonated OH and the nitrogen atom of the quinoline ring. The complexes have been characterized by elemental analyses, infrared spectroscopy, ^{1}H, ^{13}C NMR spectroscopy, mass spectrometry, and thermogravimetric analysis. The results have been supported by DFT studies using B3LYP basis set at 3-21G level.

MATERIALS AND METHODS

Materials and Physical Measurements: All the syntheses were carried out under a dry nitrogen atmosphere using a vacuum glassline. The organic solvents used were dried and purified according to standard procedures. 8-hydroxyquinoline (Himedia), silicon tetrachloride (Merck), absolute ethanol (CYC China), isopropanol (Himedia), 2,2′,2″-nitrilotriacetic acid (Aldrich), phenytrichlorosilane (Aldrich), potassium isothiocyanate (Aldrich), N-methyldiethanolamine and catechol (Aldrich) were used as supplied. Tris(2-hydroxy-3,5-dimethylbenzyl)amine[28] and chlorotriethoxysilane[29] were synthesized according to reported procedures. Infrared spectra were obtained as Nujol mulls as a KBr pellet on a Perkin–Elmer RX-I FT IR spectrophotometer. The solution ^{1}H (300 MHz), ^{13}C (75.45 MHz) NMR spectra were recorded on a Jeol and Bruker FT NMR (AL 300 MHz) spectrometer. Chemical shifts in ppm were determined relative to internal DMSO-d_6/$CDCl_3$ and external tetramethylsilane (TMS). The C, H, N and S analysis were obtained on a FLASH-2000 Organic Elemental Analyzer. The mass spectral measurements (TOF MS ES+ 1.38 eV) were carried out with a VG Analytical (70-S) spectrometer. The mass percent composition of sulfur, silicon and chlorine was determined by standard gravimetric methods. The quantum mechanical calculations were carried out using the GAUSSIAN 03 series of programs. Geometries were fully optimized at Density Functional Theory level (DFT), using Becke's three parameter hybrid exchange functional and the correlation functional of Lee, Yang, and Parr (B3LYP) with 3-21G basis set.

Thermogravimetric analyses: The TGA analysis was run on a SDT Q600 V20.9 Build 20 TGA Instrument. The sample was loaded in an alumina pan and ramped at 10°C/min over a temperature range of 25-1000°C in dry air at 60 mL min^{-1}.

Synthesis

8-(triethoxysilyloxy)quinoline (1) : The potassium salt of 8-hydroxyquinoline was prepared by dissolving 8- hydroxyquinoline (1.00 g, 6.88 mmol) and potassium hydroxide pellets (0.38 g, 6.88 mmol) in isopropanol (30 mL). The mixture was refluxed for 2 h. The yellow salt obtained was separated by filtration, and dried in *vacuo*. Chlorotriethoxysilane (1.00 g, 5.03 mmol) was added drop wise to a stirred solution of the potassium salt of 8-hydroxyquinoline (0.73 g, 5.03 mmol) in tetrahydrofuran (30 mL). The reaction mixture was stirred at room temperature for 20 h. The resulting precipitate was filtered and washed with tetrahydrofuran (2 mL). The solvent of the filtrate (including the wash solution) was removed in *vacuo*, followed by addition of diethylether (2 mL). The resulting yellow solid was isolated by filtration, washed with diethylether (2 mL) and dried in *vacuo*. Yield: 1.14 g (74%), mp 200°C (dec); IR (υ_{max}, cm^{-1}): 575 (ν(as)N→Si), 1078 (ν(as)Si-OC), 1295 (ν(as)C-O), 1594 (ν(as)C=N), 1460 (ν(as)C=C). ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.2 (t, 9H, CH_3), 3.8 (q, 6H, OCH_2), 7.1-8.7 (m, 6H, ArH); ^{13}C NMR (75.45 MHz, $CDCl_3$): δ 18.0 (CH_3), 59.1 (OCH_2), 110.0, 117.8, 121.8, 121.8, 127.8, 136.2, 138.2, 147.8, 152.2 (ArC); Anal. Calc. for $C_{15}H_{21}NO_4Si$: C, 58.63; H, 6.84; N, 4.56; Si, 9.12. Found: C, 58.60; H, 6.82; N, 4.53; Si, 9.10; MS: m/z (assignment): 308 $[M+H]^+$.

8-(dichloro(phenyl)silyloxy)quinoline (2): Phenyltrichlorosilane (1.91 g, 9.05 mmol) was added drop wise to a stirred solution of 8-hydroxyquinoline (1.31 g, 9.05 mmol) and triethylamine (0.91 g, 9.05 mmol)

in tetrahydrofuran (30 mL), and the reaction mixture was allowed to stir for 24 h. The compound **(2)** was isolated analogous to compound **(1)**. Yield: 2.05 g (72%), mp 180°C (dec); IR (υ_{max}, cm^{-1}): 515 (ν(as)N→Si), 1113 (ν(as)Si-OC), 569 (ν(as)Si-Cl), 1303 (ν(as)C-O), 1594 (ν(as)C=N), 1463 (ν(as)C=C); ^{1}H NMR (300 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 7.2-8.9 (m, 11H, ArH); ^{13}C NMR (75.45 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 115.3, 116.5, 120.3, 125.8, 127.6, 128.4, 129.1, 132.5, 132.6, 132.7, 141.9, 144.8, 147.5 (ArC); Anal. Calc. for $C_{15}H_{11}Cl_2NOSi$: C, 56.25; H, 3.43; N, 4.37; Cl, 22.18; Si, 8.75. Found: C, 56.23; H, 3.40; N, 4.34; Cl, 22.14; Si, 8.70; MS: m/z (assignment): 321 $[M+H]^+$, 359 $[M + K]^+$.

8-(nitrilotriacetatosilyloxy)quinoline (3): To a dried 100 mL two-neck round-bottom flask fitted with Dean Stark apparatus, compound **(1)** (0.80 g, 2.60 mmol) and 2,2′,2″-nitrilotriacetic acid (0.66 g, 2.60 mmol) were added in acetonitrile (30 mL). The contents were refluxed for 5 h. The resulting yellow solid was isolated by filtration, washed with acetonitrile (5 mL) and dried in *vacuo*. Yield: 0.74 g (79%), mp 220°C (dec); IR (υ_{max}, cm^{-1}): 576, 621 (ν(as)N→Si), 1095 (ν(as)Si-OC), 1300 (ν(as)C-O), 1727 (ν(as)C=O), 1596 (ν(as)C=N), 1462 (ν(as)C=C); ^{1}H NMR (300 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 3.5 (s, 6H, NCH_2), 7.4-7.9 (m, 6H, ArH); ^{13}C NMR (75.45 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 54.7 (NCH_2), 171.6 (C=O), 114.5, 117.6, 117.7, 121.4, 129.2, 129.3, 142.8, 144.4, 149.7 (ArC); Anal. Calc. for $C_{15}H_{12}N_2O_7Si$: C, 50.00; H, 3.33; N, 7.77; Si, 7.77. Found: C, 49.96; H, 3.31; N, 7.76; Si, 7.75; MS: m/z (assignment): 361 $[M+H]^+$.

1-(quinolin-8-yloxy)-2,8,11-trioxa-6-aza-1-sila-3,4;8,9;12,13-tris(4,6-dimethylbenzo) [4.4.4] tricycle tetradecane(4): To a dried 100 mL two-neck round-bottom flask fitted with Dean Stark apparatus, compound **(1)** (1.00 g, 3.25 mmol) and tris(2-hydroxy-3,5-dimethylbenzyl)amine (1.36 g, 3.25 mmol) were added in dichloromethane (30 mL). The contents were refluxed for 5 h. The solvent of the clear solution obtained was removed in *vacuo*, followed by addition of diethylether (2 mL). The resulting yellow solid was isolated by filtration, washed with diethylether (2 mL) and dried in *vacuo*. Yield: 1.43 g (75%), mp 260°C (dec); IR (υ_{max}, cm^{-1}): 518, 575 (ν(as)N→Si); 1108 (ν(as)Si-OC), 1313 (ν(as)C-O), 1595 (ν(as)C=N), 1466 (ν(as)C=C); ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.0 (s, 18H, $ArCH_3$), 4.0 (s, 6H, NCH_2), 6.6-8.8 (m, 12H, ArH); ^{13}C NMR (75.45 MHz, $CDCl_3$): δ 56.5 (NCH_2), 19.9 ($ArCH_3$), 20.0 ($ArCH_3$), 96.2, 108.8, 112.5, 115.8, 116.3, 118.2, 120.1, 121.6, 124.7, 129.8, 130.2, 131.5, 134.2, 146.4, 149.9 (ArC); Anal. Calc. for $C_{36}H_{36}N_2O_4Si$: C, 73.46; H, 6.12; N, 4.76; Si, 4.76. Found: C, 73.42; H, 6.09; N, 4.71; Si, 4.73; MS: m/z (assignment): 588 $[M]^+$, 611 $[M + Na]^+$.

8-(diisothiocyanato(phenyl)silyloxy)quinoline (5): To a stirred solution of compound (**2**) (1.00 g, 3.12 mmol) in acetonitrile (30 mL), potassium isothiocyanate (0.60 g, 3.12 mmol) was added and the reaction mixture was allowed to stir for 24 h. The KCl was filtered and washed with acetonitrile (3 mL). The compound was isolated analogous to compound **(3)** except that hexane (2 mL) was added instead of ether. Yield: 0.85 g (75%), mp 172°C; IR (υ_{max}, cm^{-1}): 580 (ν(as)N→Si), 1134 (ν(as)Si-OC), 1310 (ν(as)C-O), 2085 (ν(as)NCS), 1587 (ν(as)C=N), 1463 (ν(as)C=C); ^{1}H NMR (300 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 7.2-9.0 (m, 11H, ArH); ^{13}C NMR (75.45 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 114.3, 114.3, 117.3, 117.4, 121.2, 127.0, 129.1, 129.4, 142.6, 143.8, 143.8, 149.6, 149.6 (ArC), 133.8 (NCS); Anal. Calc. for $C_{17}H_{11}N_3OS_2Si$: C, 55.89; H, 3.01; N, 11.50; S, 17.53; Si, 7.67. Found: C, 55.86; H, 2.98; N, 11.48; S, 17.50; Si, 7.65; MS: m/z (assignment): 367 $[M+2H]^{2+}$.

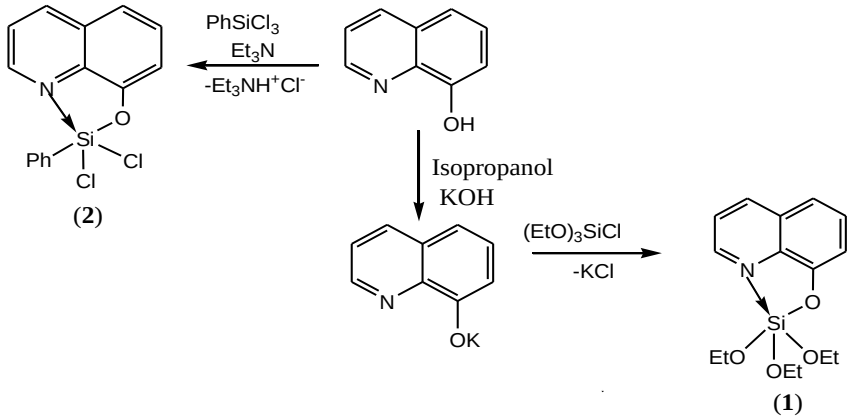
8-(2-phenylbenzo-1,3,2-dioxasilol-2-yloxy)quinoline (6): To a stirred solution of compound **(2)** (1.0 g, 3.12 mmol) and triethylamine (0.87 g, 6.25 mmol) in tetrahydrofuran (30 mL), catechol (0.34 g, 3.12 mmol) was added and the reaction mixture was allowed to stir for 24 h. The compound was isolated analogous to compound **(3)**. Yield: 0.89 g (80%), mp 230°C (dec); IR (υ_{max}, cm^{-1}): 525 (ν(as)N→Si), 1111 (ν(as)Si-OC), 1299 (ν(as)C-O), 1597 (ν(as)C=N), 1468 (ν(as)C=C); ^{1}H NMR (300 MHz, $CDCl_3$/CCl_4): δ 6.6-8.6 (m, 15H, ArH); ^{13}C NMR (75.45 MHz, $CDCl_3$/CCl_4) δ 110.4, 110.9, 115.9, 117.6, 119.0, 120.6, 121.6, 127.3, 127.9, 128.6, 134.5, 136.3, 144.4, 147.5, 149.5, 152.4 (ArC); Anal. Calc. for $C_{21}H_{15}NO_3Si$:

C, 70.58; H, 4.20; N, 3.92; Si, 7.84. Found: C, 70.56; H, 4.19; N, 3.91; Si, 7.82; MS: m/z (assignment): 360 $[M+3H]^{3+}$.

8-(6-methyl-2-phenyl-1,3,6,2-dioxazasilocan-2-yloxy)quinoline (7): To a stirred solution of compound **(2)** (1.0 g, 3.12 mmol) and triethylamine (0.63 g, 6.25 mmol) in tetrahydrofuran (30 mL), N-methyldiethanolamine (0.37 g, 3.12 mmol) was added dropwise and the reaction mixture was allowed to stir for 24 h. The compound was isolated analogous to compound **(3)**. Yield: 0.82 g (72%), mp 210°C (dec); IR (υ_{max}, cm^{-1}): 537, 576 (ν(as)N→Si), 1093 (ν(as)Si-OC), 1299 (ν(as)C-O), 1595 (ν(as)C=N), 1454 (ν(as)C=C); ^{1}H NMR (300 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 2.5 (s, 3H, CH_3), 2.8 (t, 4H, NCH_2), 3.6 (t, 4H, OCH_2), 7.0-8.7 (m, 11H, ArH); ^{13}C NMR (75.45 MHz, DMSO-d_6/$CDCl_3$/CCl_4): δ 45.2 (CH_3), 58.2 (OCH_2), 56.4 (NCH_2), 110.1, 117.1, 117.9, 121.1, 123.4, 126.6, 127.0, 128.2, 133.5, 135.4, 138.1, 147.2, 152.5 (ArC); Anal. Calc. for $C_{20}H_{22}N_2O_3Si$: C, 65.57; H, 6.01, N, 7.65; Si, 7.65. Found: C, 65.55; H, 6.00; N, 7.63; Si, 7.62; MS: m/z (assignment): 367 $[M+H]^+$.

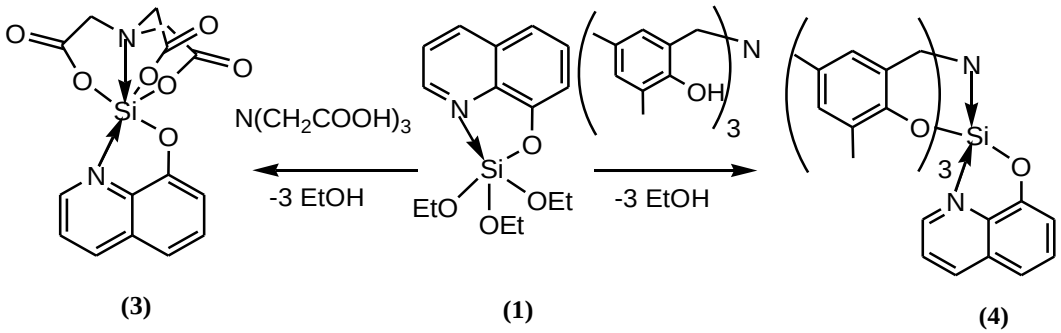
RESULTS AND DISCUSSION

Synthesis : 8-(triethoxysilyloxy)quinoline (**1**) was prepared by the reaction of the potassium salt of 8-hydroxyquinoline with chlorotriethoxysilane and 8-(dichloro(phenyl)silyloxy)quinoline (**2**) was synthesized by the reaction of 8-hydroxyquinoline with phenytrichlorosilane using triethylamine as a base scavenger as shown in scheme 1.



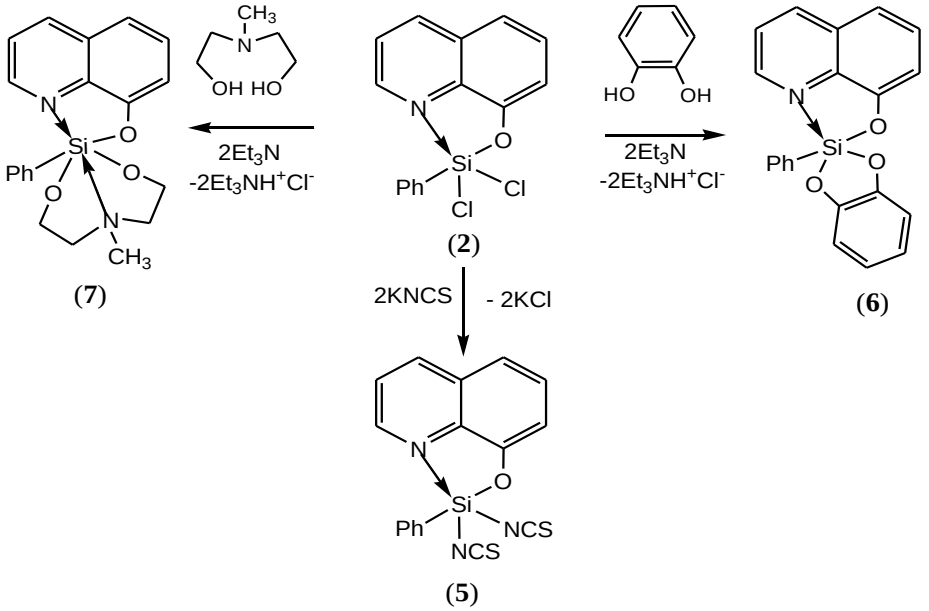
Scheme 1

Silatranes (**3-4**) were obtained by the transesterification of (**1**) with tripodal ligands such as 2,2′,2″-nitrilotriacetic acid and tris(2-hydroxy-3,5-dimethylbenzyl)amine respectively as shown in scheme 2.



Scheme 2

The reactions of complex (**2**) with potassium isothiocyanate, catechol and N-methyldiethanolamine led to the formation of hypervalent complexes (**5-7**) respectively (Scheme 3). The composition of the complexes was confirmed by their analytical data and the structures were supported by the spectroscopic investigations.



Scheme 3

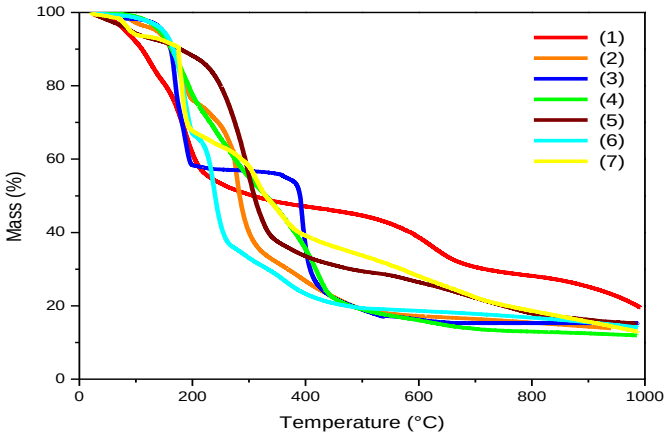
IR Spectra: The coordination of oxygen and nitrogen atoms of the quinoline to silicon was pursued by IR spectra by comparing the spectra of the complexes with that of free ligand[30]. Absence of a band at 3300 cm^{-1} due to ν(OH) of free 8-hydroxyquinoline in the IR spectra of the complexes confirmed that the phenolic oxygen atom was coordinated to the silicon. The bonding of the phenolic oxygen atom to silicon was supported by the fact that the Si–O band appeared in the expected region 1078-1113 cm^{-1} and the most important characteristic absorption bands associated with these structures operating in the region 525-580 cm^{-1} were assigned to N→Si. A strong band observed at 1276 cm^{-1} in the spectrum of the ligand, which was attributed to the phenolic C-O stretching vibration, underwent a shift to higher wavenumber 1295 - 1310 cm^{-1} in the spectra of the complexes. In the spectra of analyzed complexes, the absorption band assigned for the *ν*(C=N) of quinoline group was shifted to lower region 1594-1597 cm^{-1} as compared to spectrum of the free ligand. Thus, the infrared spectra data showed that 8-hydroxyquinoline acted as a bidentate ligand and coordinated through the nitrogen atom and was covalently bonded through phenolic oxygen to silicon. In complex (**3**), the band corresponding to carboxyl group appeared at 1727 cm^{-1}. The IR spectrum of complex (**5**) showed a strong NCS band at 2085 cm^{-1}.

NMR Spectra: Multinuclei (^1H and ^{13}C) NMR spectra were consistent with the structure of synthesized complexes. The disappearance of broad singlet signal due to the OH proton in the spectra of complexes suggested deprotonation of phenolic group and its subsequent involvement in the coordination. In particular, broadening or coordination induced shifts of the ^1H and ^{13}C signals of the ligand on complexation, when compared with those of the free ligand, gave clear indications of the ligand-to-silicon atom coordination. In ^1H NMR spectrum of the complex (**1**), signals of OCH_2 and CH_3 protons appeared at 3.8 and 1.2 ppm respectively. On comparing the ^1H and ^{13}C NMR spectra of the complex (**4**) with that of the ligand tris(2-hydroxy-3,5-dimethylbenzyl)amine, a downfield shift for the protons and carbon atoms of the -CH_2N- moiety in all compounds was observed. In complex (**7**), NCH_2 and OCH_2 signals were observed as a triplet at 2.8 and 3.6 ppm respectively while the CH_3 protons appeared as a singlet at 2.5 ppm. Overall, the resonances in the pyridyl ring and phenoxide ring of the complexes shifted downfield with respect to that of the free ligand[31]. In ^{13}C NMR spectra of complex (**1**), signals corresponding to

OCH_2 and CH_3 appeared at 59.1 and 18.0 ppm respectively. The complexes (**3**) and (**4**) showed signals corresponding to NCH_2 at 54.7 and 56.5 ppm respectively. The spectra of complexes displayed distinct ^{13}C signals for the aromatic carbon atoms in all the cases. The ^{13}C NMR spectra of (**3**) and (**5**) displayed signals at 171.6 and 133.8 ppm corresponding to the carbon atom of the carbonyl and NCS group respectively. In complex (**7**), NCH_2 and OCH_2 were observed at 56.4 and 58.2 ppm respectively. The CH_3 carbon appeared at 45.2 ppm.

Mass Spectra: The mass spectra of all the compounds showed the molecular ion peaks, quasi molecular ion peaks with addition of H^+ and K^+ ions which were consistent with the molecular masses of the individual compounds. In all the compounds, the peak at m/z = 146 corresponded to protonated 8-hydroxyquinoline ligand.

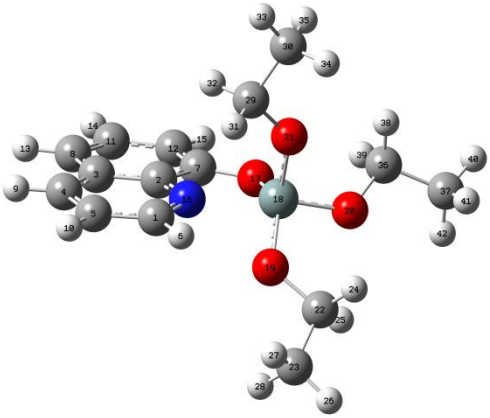
Thermogravimetric analysis: The thermal stability of all the silicon compounds was studied by thermogravimetric analysis (Fig. 1).



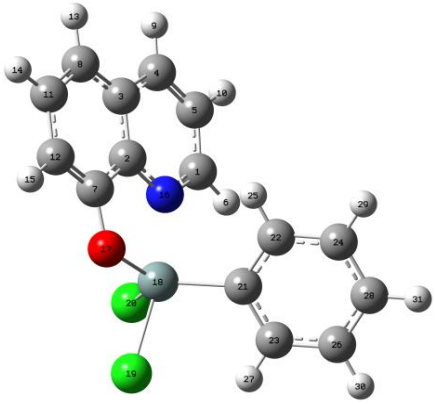
The complexes were heated from 25 to 1000 °C under nitrogen atmosphere. The first step of the TGA curve of compound (**1**) was attributed to the loss of ethoxy group (calc = 14.33%, expt = 14.65%) until 172°C and the next step involved the decomposition of the rest of the molecule and the residue corresponded to the formation of SiO_2 (calc = 19.43%, expt = 19.56%). The TGA curve of compound (**2**) revealed the loss of chlorine atoms (calc = 23.76%, expt =22.18%) in the temperature range of 170-220 °C. The second step was attributed to the decomposition of rest of the molecule while the residue corresponded to the formation of SiO_2 (calc = 17.23%, expt = 18.75%). In the TGA curve of compound (**3**), initially the loss of 8-hydroxyquinoline moiety did not occur until 200 °C (calc = 41.11%, expt = 40.27%) and the next step showed the weight loss of the rest of the molecule leaving SiO_2 (calc = 16.12%, expt = 16.66%) as residue at the end of degradation process. In compound (**4**), the first step corresponded to the loss of the 8-hydroxyquinoline moiety (calc = 24.23%, expt = 24.65%) and the subsequent steps accounted for the decomposition of the complex while the residue corresponded to the formation of SiO_2 (calc = 11.57%, expt = 10.20%).The compound (**5**) showed the loss of NCS group (calc = 15.85%, expt =16.46%) initially and at 280 °C the decomposition of the rest of the molecule followed and the residue corresponded to the formation of SiO_2 (calc = 15.59%, expt = 15.98%). In the TGA curves of (**6**), the initial loss of catechol (calc = 31.23%, expt = 31.83%) occurred at 230 °C following the complete decomposition of the rest of the molecule while the residue corresponded to the formation of SiO_2 (calc = 16.28%, expt = 16.80%). The TGA curves of (**7**), the initial loss of N-methyldiethanolamine (calc = 31.83%, expt = 32.51%) was

observed following the decomposition of the complex in subsequent steps leaving SiO_2 as the residue (calc = 15.73%, expt = 16.39%).

Computational Study: The geometries of all structures reported herein (Fig. 2) were optimized by density functional theory[32] (DFT) using B3LYP[33] along with the 3-21G basis set which has proven its utility for describing accurate geometrical features. All DFT optimizations were preformed with the Gaussian 03 set of programs.



(1)



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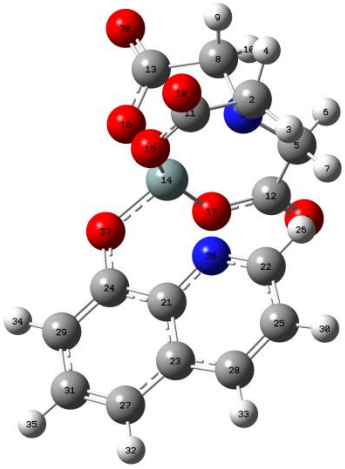

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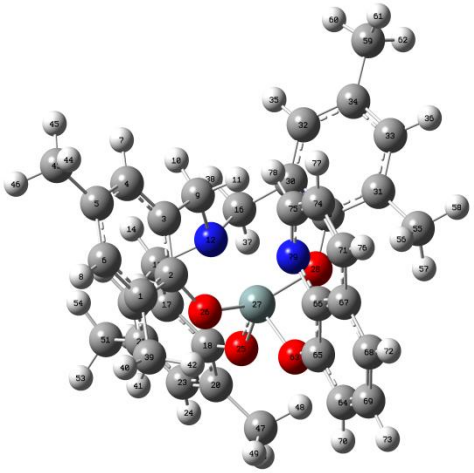

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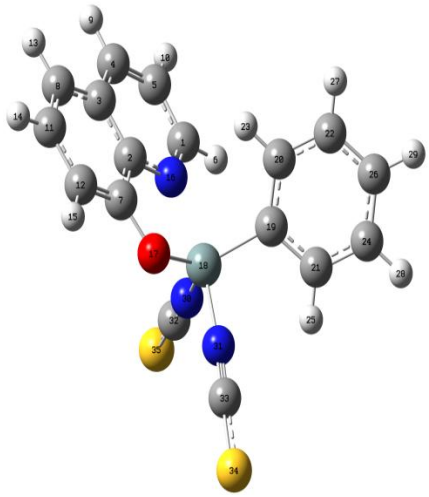

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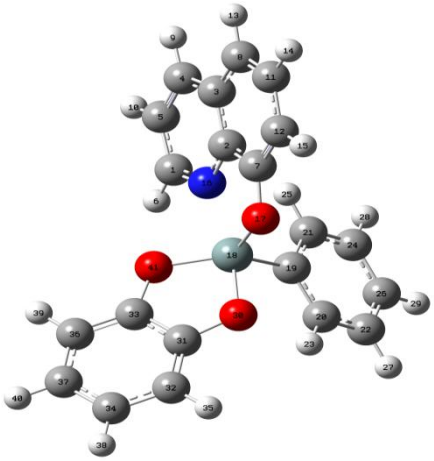
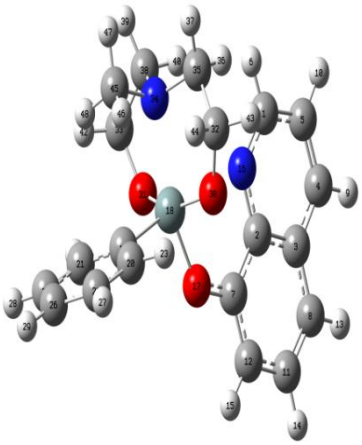


(6)



(7)

Fig. 2: Optimized structures of complexes (1-7)

The optimized geometrical parameters of the synthesized compounds have been summarized in table 1.

Table 1. Parameters of optimized structures of complexes **(1-7)** using DFT method

Parameter	**(1)**	**(2)**	**(3)**	**(4)**	**(5)**	**(6)**	**(7)**
Energy[a]	-1222.91	-1908.44	-1504.60	-2082.25	-1711.36	-1371.85	-1392.58
Dipole moment[b]	6.06	10.95	5.34	8.78	6.65	7.39	6.80
N→Si[c]	2.07	2.06	2.20, 2.13	2.06, 2.66	2.10	2.04	2.19, 2.79
Si-O av.	1.72	1.76	1.72	1.72	1.75	1.76	1.73

[a] In (a.u.) [b] In (Debye) [c] In (Å)

The most intriguing aspect of the higher-coordinate silicon complexes is the nature of the silicon-nitrogen interaction. The silicon-nitrogen internuclear distance (N→Si) in all the optimized structures was found in the range 2.04-2.79 Å. These distances were considerably shorter than the sum of the van der Waals radii of 3.50 Å for silicon and nitrogen, yet the distances were longer than a conventional silicon-nitrogen covalent bond length of 1.86 Å found in tetra-coordinate silicon compounds. This clearly indicated that the higher coordination based on N→Si distances of experimentally (IR, NMR, MS) suggested structures (**1-7**) have been complemented by DFT computations. The Si-O av. distances in all the complexes were ranging from 1.72-1.76 Å. The silicon-coordination polyhedral of the penta-coordinate silicon(IV) complexes (**1**,**2**,**5,6**) were distorted trigonal bipyramids whereas the silicon-coordination polyhedral of the hexa-coordinate silicon(IV) complexes (**3**,**4**,**7**) were best described as a distorted octahedron.

APPLICATIONS

The prepared complexes have applications in the field of biology, material science, pharmaceutics, agriculture, etc.

CONCLUSIONS

To examine the versatility of formation of higher coordinate silicon compounds via silicon-nitrogen donor action, we synthesized, characterized and studied the reactivity of higher-coordinate complexes of silicon with 8-hydroxyquinoline. Systematic studies on compounds of this type could further our understanding of the influence of different types of ligand atoms on the bonding situation at penta- and hexa coordinate silicon centers, and they offer other new perspectives for the chemistry of higher coordinate silicon based on their structural properties, reactivity and applications in the field of biology, material science, pharmaceutics, agriculture, etc.

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