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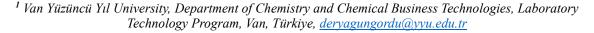
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SYNTHESIS AND ELECTRONIC PROPERTIES OF AXIALLY **DISUBSTITUTED SILICON (IV) PHTHALOCYANINE 9-**PHENYL-9H-XANTHENE-9-OXY

Derya GÜNGÖRDÜ SOLĞUN ¹ 🕩



ABSTRACT

In this research, a new axial phthalocyanine complex compound was synthesized. This study involved the synthesis of the novel silicon phthalocyanine prepared by reacting SiPcCl₂, 9phenyl-9H-xanthen-9-ol and K₂CO₃ in dry toluene. The novel silicon phthalocyanine was characterized by using different spectroscopic techniques including 1H NMR, UV-Visible, FT-IR and mass spectroscopy. The electronic properties of the compound for example the aggregation and solubility parameters investigated. Aggregation is a crucial parameter dictating the functional performance of phthalocyanines. Aggregation is closely related to temperature, concentration, type of ligand attached to the phthalocyanine ring, substituents attached to peripheral positions and polarity of the solvent. Ligands attached to the phthalocyanine ring disrupt the planarity of the ring, resulting in reduced aggregation. For these reasons, in this study, we focused on the aggregation characteristics of phthalocyanines and how axial ligand modifications regulate this behavior. Axial ligand (especially those with metals like Si, Ge, Sn) coordination increases steric bulk and reduces stacking. The low aggregation tendency of phthalocyanines provides significant advantages, especially in photodynamic therapy (PDT), optoelectronics and sensor applications. Photodynamic therapy (PDT) is a light based therapeutic modality that requires the coordinated presence of three key components: a photosensitizer (PS), a light source, and molecular oxygen. Phthalocyanine based photosensitizers (Pcs) are among the most promising candidates for photodynamic therapy (PDT) due to their favorable photophysical and photochemical properties. An ideal photosensitizer should exhibit strong absorption (600–800 nm), where tissue penetration of light is optimal. Phthalocyanines meet this criterion through their intense Q band absorption, usually around 670–700 nm. Moreover, they are capable of efficiently generating singlet oxygen ($\Phi\Delta$), a key cytotoxic agent in PDT. In addition to their photodynamic efficiency, phthalocyanines demonstrate excellent chemical and photostability.

Preliminary research was conducted for photosensitizer properties of the compound. After researches, the results have showed that singlet oxygen quantum yield has increased in the photodynamic study ($\Phi\Delta$ =0.19) compare to the Std-SiPc ($\Phi\Delta$ = 0.15)

Keywords: Silicon phthalocyanine, Synthesis, Singlet oxygen, Electronic properties,

Aggregation.

1 INTRODUCTION

Phthalocyanines (Pcs) which is aromatic macrocyclic compounds in coordination chemistry have high conjugation. Pcs consist of a 16-membered (8 carbon, 8 nitrogen) planar macrocycle with an $18-\pi$ electron system. The most important factor affecting the solubility of phthalocyanines is the strong π interactions between phthalocyanine molecules. As the π -stacking is prevented, the solubility of phthalocyanines in different solvents is increased. By adding axial ligands to the central metal atom (Si, Al, Ge, Ti, Sn, etc.), the solubility can be increased by reducing the π interaction between molecules.

Due to the electronic delocalization of phthalocyanines, they have been found to be useful for many applications in different fields. It is well known by scientists that phthalocyanines have been investigated in a wide range. These compounds research or usage areas can be listed as catalysts [1-2], electrochromics [3], photovoltaics [4-5], non-linear optics [6-7], dyes [8], antioxidants [9-10], antifungals [11], antibacterials [12], photosensitizers, sonosensitizers for photodynamic therapy [13-15], liquid crystals [16], gas sensors [17], thermal stabilities [18] or metal ion sensors [19-20]. Cancer is a disease that has been increasing worldwide recently and is being treated in different combinations [21]. Photodynamic therapy (PDT), which is an alternative treatment method to chemotherapy and radiotherapy, which are traditional methods used in the fight against this disease, is attracting attention [22]. PDT is based on the irradiation of the photosensitizer (PS) compound with light in the presence of oxygen. Phthalocyanines are complexes with high absorption coefficients in the 600-800 nm region [23]. The light used in PDT is usually in the range of 650-850 nm, which allow light to pass through human tissues. After light irradiation, energy is transferred from the photosensitizer to elemental oxygen and singlet oxygen is produced. After this production, singlet oxygen damages the DNA of cancer cells and can cause cell death [24-25]. The use of low-energy light and few side effects makes PDT more advantageous than other cancer treatment methods [26]. This treatment offers the patient comfort and deeper tissue penetration. For these purposes, it is aimed to synthesize new phthalocyanines and to reveal the photosensitizer potential of the synthesized compound.

In this study, a new bis(9-phenyl-9H-xanthen-9-oxy) phthalocyaninato silicon (IV) compound was synthesized and characterized. Additionally, the spectroscopic and photochemical properties of the phthalocyanine complex were investigated to determine their potential as photosensitizer in photodynamic therapy.

2 MATERIAL AND METHOD

Chloroform (CHCl₃), tetrahydrofuran (THF), dimethylformamide (DMF), and dimethyl sulfoxide (DMSO) were purchased from Sigma-Aldrich. SiPcCl₂ and 9-phenyl-9H-xanthen-9-ol were supplied by Alfa Aesar. Potassium carbonate (K₂CO₃), methanol, dichloromethane (CH₂Cl₂), and toluene were supplied by Merck and Acros Organics respectively. For structure characterization of UV visible spectra a Hitachi U-2900 Spectrophotometer was used. A Thermo Scientific FT-IR spectrometer was used to determine the vibration bands. NMR spectra were determined with an Agilent 400 MHz NMR spectrometer. Mass analysis of the compound was performed using an LC-MS electrospray.

2.1 Synthesis

Bis(9-phenyl-9H-xanthen-9-oxy) phthalocyaninato silicon (IV) (1)

SiPcCl₂ (75 mg, 0.12 mmol), 9-phenyl-9H-xanthen-9-ol (132 mg, 0.48 mmol) and K₂CO₃ (55 mg, 1.43 mmol) were mixed in dry toluene (10 mL) and refluxed for 24 h. Then the mixture has cooled to room temperature, the organic phase was separated by extraction (chloroform: water). After evaporation of solvent, the product was obtained. The product was dissolved in THF. Purification steps included by washing with ethanol and methanol. After this step, the product was dissolved in CH₂Cl₂ and filtered again. Finally, CH₂Cl₂ solutes were taken. m.p. > 300°C. Yield: 33 mg (25 %), FTIR (ATR), v/cm⁻¹: 3053 (Ar-H), 1602 (C=N), 1571-1479 (Ar-C=C), 1450, 1315 (C-N), 1265, 1246-1151 (Ar-O-Ar), 1099-1070 (Si-O-C), 1033, 894, 871, 732, 704, 628. ¹H NMR (400MHz, DMSO-d₆), (δ): 7.35, 7.34, 7.31, 7.27, 7.24, 7.13, 7.09, 6.76. UV–Vis (CH₂Cl₂, 1×10⁻⁵ M): λ max/nm (log ϵ): 675 (5.17), 350 (4.86). MS (ESI), (m/z): Calculated for C₇₀H₄₂N₈O₄Si: 1086.3; Found:1087 [M+H]⁺.

3 RESULTS AND DISCUSSION

The synthesis method of phthalocyanine 1 is given in Figure 1. This compound is soluble in tetrahydrofuran, chloroform, dichloromethane, N,N-dimethylformamide, dimethyl sulphoxide. After the synthesis of the phthalocyanine, purification processes were carried out. Then the characterization process was started. In the IR spectrum of phthalocyanine 1 was observed aromatic vibrations at 3086 cm⁻¹, C=N peak was observed at 1602, the C=C peaks peak was observed at 1571-1479 cm⁻¹, C-N peak was observed at 1315, Ar-O-Ar bond

vibrations was observed at 1246-1151, Si-O-C stretch peak was observed at 1099-1070 cm⁻¹ which was supported data in the literature [27].

In the ESI mass spectrometry gived ion peak at 1087 [M+H]⁺ which was the expected.

In the ¹H NMR spectrum of compound **1**, aromatic protons were located at in the range of 7.35-6.76 ppm support the structure.

Figure 1. Synthesis scheme of compound 1.

The absorbance values saw in the UV-visible spectrum of the phthalocyanine complex are the Q band at 675 nm and the B band at 350 nm. These values are consistent with the absorbance values expected for the phthalocyanine structure. Electronic measurements of the compound in the range of 1.4×10^{-5} - 0.2×10^{-6} M show that the compound is not aggregated (Figure 2). These observed values show that the compound meets the prerequisite for use as a photosensitizer. If further studies support this parameter, the compound can be used as a photosensitizer.

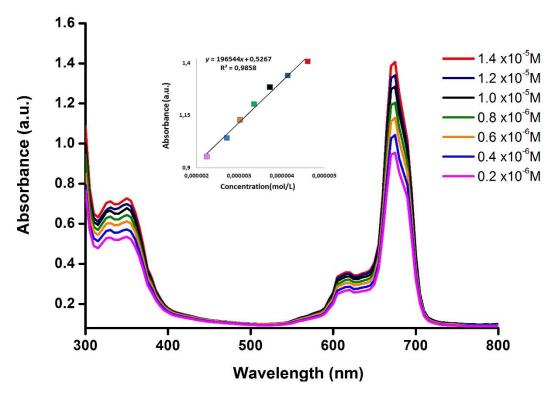


Figure 2. Absorption spectra of compound 1 in CH2Cl2 at 1.4x10-5- 0.2x10-6M concentrations.

The electronic absorption of compound 1 in tetrahydrofuran, chloroform, dichloromethane, N,N-dimethylformamide, dimethyl sulphoxide is shown in Figure 3. This compound is easily dissolved this solvents.

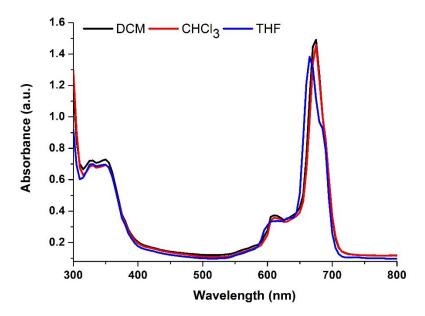


Figure 3. Absorption spectra of compound 1 in dichloromethane, chloroform and tetrahydrofuran solvents.

Phthalocyanines are interesting with their singlet oxygen production capacity. A quality sensitizer should have a great singlet oxygen efficiency. The light used in this study was provided by a 150 volt lamp. The sample was then exposed to light passed through an optical filter with a wavelength range of 650-720 nm, and placed in the cuvette. The singlet oxygen quantum yield of compound 1 was measured at 417 nm. DPBF was dissolved in DMSO under dark conditions, and the sample was subsequently irradiated within the Q band absorption region. The degradation of DPBF at 417 nm was monitored after each 5 s illuminate. While the Q bands of 1 did not alter, DPBF absorbance was decreased (Figure 4). Compound 1 has a high value (Φ_{Δ} = 0.19) than Std-SiPc (Φ_{Δ} = 0.15) [28].

Singlet oxygen quantum yield (Φ_{Δ}) , a critical parameter in evaluating a photosensitizer's efficiency in photodynamic therapy, is typically calculated using a relative method with a standard reference photosensitizer. The singlet oxygen quantum yield (Φ_{Δ}) of a photosensitizer was determined by a comparative method using a reference compound with a known Φ_{Δ} value. The Φ_{Δ} value was calculated according to the equation:

$$\Phi_{\Delta} = \Phi_{\Delta}^{\text{Std}} \times \frac{R}{R_{\text{Std}}} \times \frac{I_{\text{abs}}^{\text{Std}}}{I_{\text{abs}}}$$
 (1)

 Φ_{Δ} : Singlet oxygen quantum yield of the sample

 $\Phi_{\Delta}^{\text{std}}$: Singlet oxygen quantum yield of the standard

R_{DPBF}: Photobleaching rate of the singlet oxygen quencher in the presence of the sample

R_{DPBF}Std: Photobleaching rate in the presence of the standard

I_{abs}: Absorbance of the sample at the irradiation wavelength

Iabs^{std}: Absorbance of the standard at the irradiation wavelength

The good performance of the phthalocyanine compound in singlet oxygen production shows that it has an advantageous effect. It shows the potential to be used in photodynamic therapy with other supportive tests.

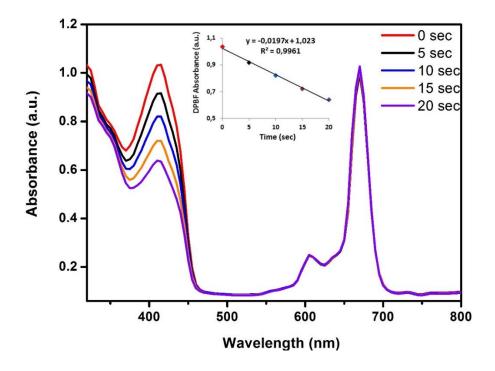


Figure 4. Measurement diagram of singlet oxygen quantum yield for compound 1.

4 CONCLUSION AND SUGGESTIONS

Bis(9-phenyl-9H-xanthen-9-oxy) phthalocyaninato silicon (IV) compound was originally synthesized. Compound 1 was characterized by ¹HNMR, UV-visible, FTIR, mass spectra. The electronic properties of bis(9-phenyl-9H-xanthen-9-oxy) phthalocyaninato silicon (IV) and its potential to produce singlet oxygen were investigated. Compound 1 show the potential to be used as a singlet oxygen generating agent for PDT.

This work has introduced a novel phthalocyanine derivative, bis(9-phenyl-9H-xanthen-9-oxy) phthalocyaninato silicon (IV), which was synthesized and characterized for the first time. The new axially disubstituted silicon(IV) phthalocyanine (Compound 1) was confirmed by comprehensive spectroscopic analysis (¹H NMR, UV-Vis, FT-IR, and mass spectrometry). Basic electronics and photochemical properties of this compound were examined in detail, with particular focus on its ability to generate singlet oxygen (¹O₂).

The results demonstrate that Compound 1 is a highly efficient singlet oxygen photosensitizer. The singlet oxygen quantum yield (Φ_{Δ}) of this new phthalocyanine was measured as 0.19 which is superior to that of a standard silicon phthalocyanine $(\Phi_{\Delta}=0.15)$. This enhanced ${}^{1}\text{O}_{2}$ generation capacity indicates a notable improvement over similar phthalocyanine compounds reported in the literature. Such performance underscores the compound's potential not only in photodynamic therapy but also in advanced multi-modal treatment approaches. In

addition to its high singlet oxygen production, the structural features of Compound 1 impart other advantages for biomedical application. The bulky 9-phenyl-9H-xanthen-9-ol ligands likely reduce π – π stacking interactions, thereby lowering the aggregation tendency and improving solubility. These traits are highly desirable for phthalocyanine-based photosensitizers in biological environments. In summary, this study not only introduces a new silicon phthalocyanine derivative to the literature, but also demonstrates its promise as an efficient singlet oxygen generator for photodynamic therapy.

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Statement of Research and Publication Ethics

The study is complied with research and publication ethics.

Artificial Intelligence (AI) Contribution Statement

This manuscript was entirely written, edited, analyzed, and prepared without the assistance of any artificial intelligence (AI) tools. All content, including text, data analysis, and figures, was solely generated by the authors.

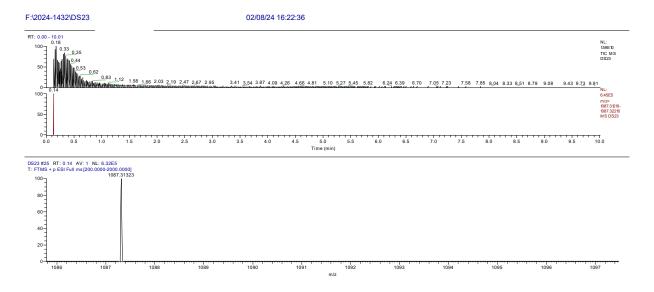
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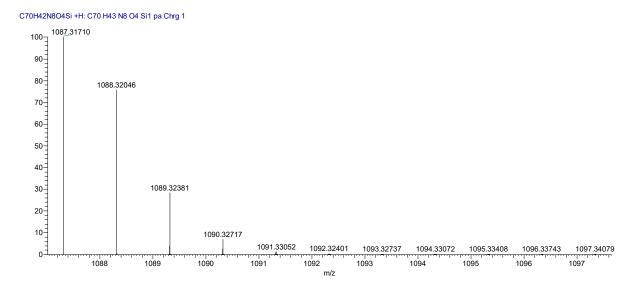
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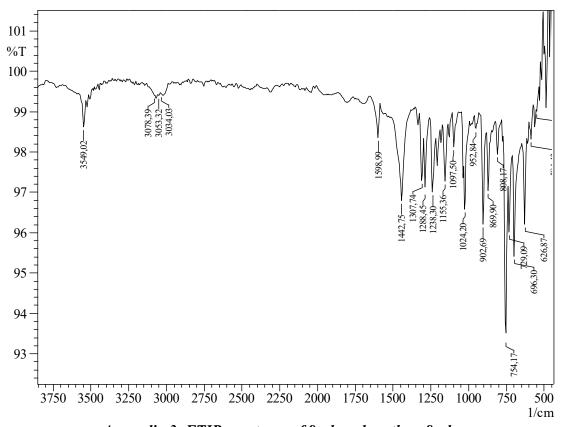
SUPPLEMETARY MATERIALS



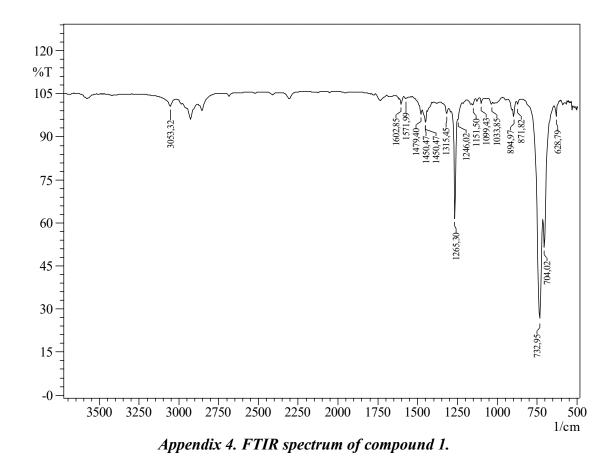
Appendix 1. HRMS (ESI) spectrum of $[M+H]^+$.

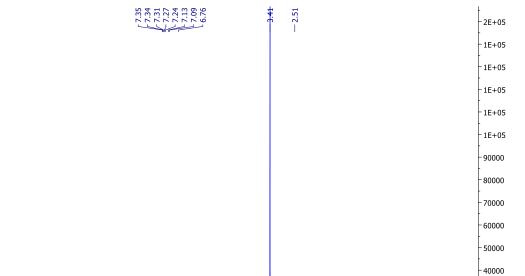


Appendix 2. HRMS (ESI) spectrum of compound 1 (Theoretical).



Appendix 3. FTIR spectrum of 9-phenylxanthen-9-ol.





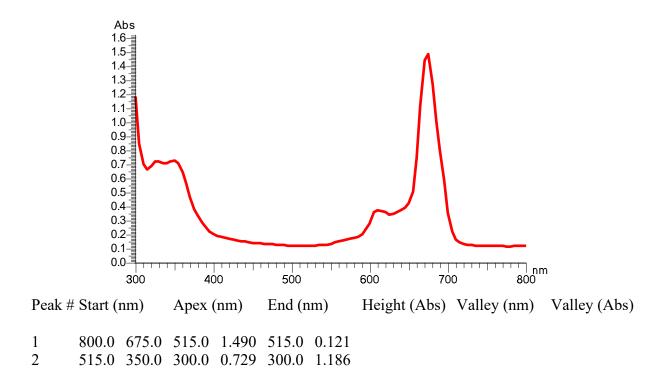
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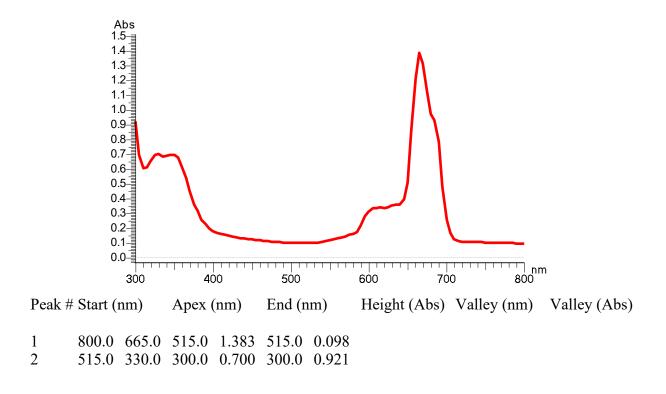
Appendix 5. ¹H NMR spectrum of compound 1.

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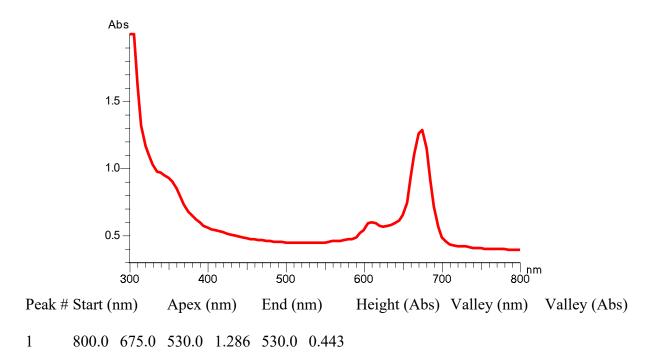
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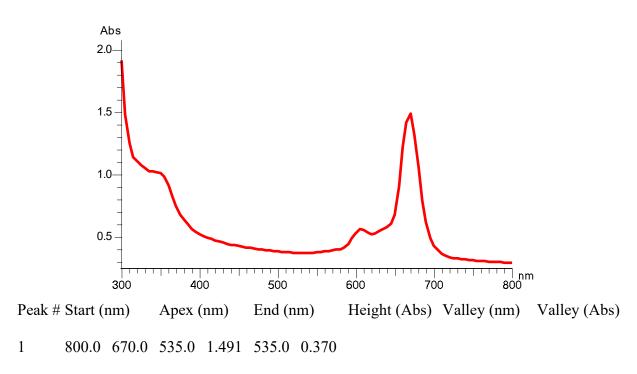
Appendix 6. UV-Vis spectrum of compound 1 in THF.



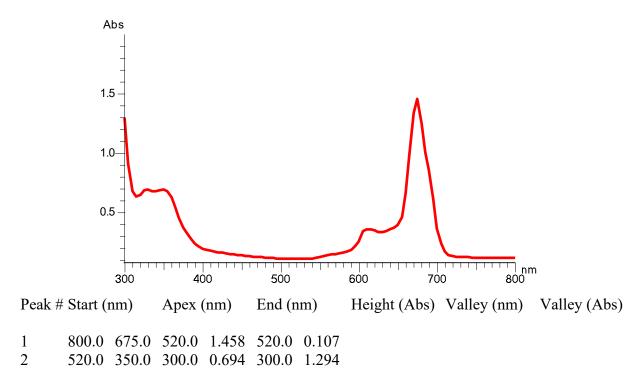
Appendix 7. UV-Vis spectrum of compound 1 in DCM.



Appendix 8. UV-Vis spectrum of compound 1 in DMSO.



Appendix 9. UV-Vis spectrum of compound 1 in DMF.



Appendix 10. UV-Vis spectrum of compound 1 in CHCl3.

Chemical Formula: C₇₀H₄₂N₈O₄Si Exact Mass: 1086,3 Molecular Weight: 1087,2

m/z: 1086.3 (100.0%), 1087.3 (75.7%), 1088.3 (28.3%), 1089.3 (6.1%), 1087.3 (5.1%), 1088.3 (3.8%), 1088.3 (3.3%), 1087.3 (3.0%), 1089.3 (2.5%), 1088.3 (2.2%), 1089.3 (1.4%), 1090.3 (1.3%) Elemental Analysis: C, 77.33; H, 3.89; N, 10.31; O, 5.89; Si, 2.58

Appendix 11. Structural analysis data of compound 1.