

Chemo-sensing and Antibacterial study of hyperordinated organo-silicon compounds

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Abstract

Organo silicon compounds which have been synthesized and already published here are used for their specific studies in the field of chemo sensor and biological active compounds. These compounds show a very high and efficient property in both these fields. They have been well characterized with the help of spectroscopic techniques which are very advanced in today's world for example proton nuclear magnetic resonance spectroscopy, carbon -13 nuclear magnetic resonance spectroscopy, infrared spectroscopy, UV spectroscopy and by mass spectroscopy. These newly compounds are also studied under elemental analytical procedure. Their chemo sensing and antibacterial studies have been studied in a micro-biological laboratory.

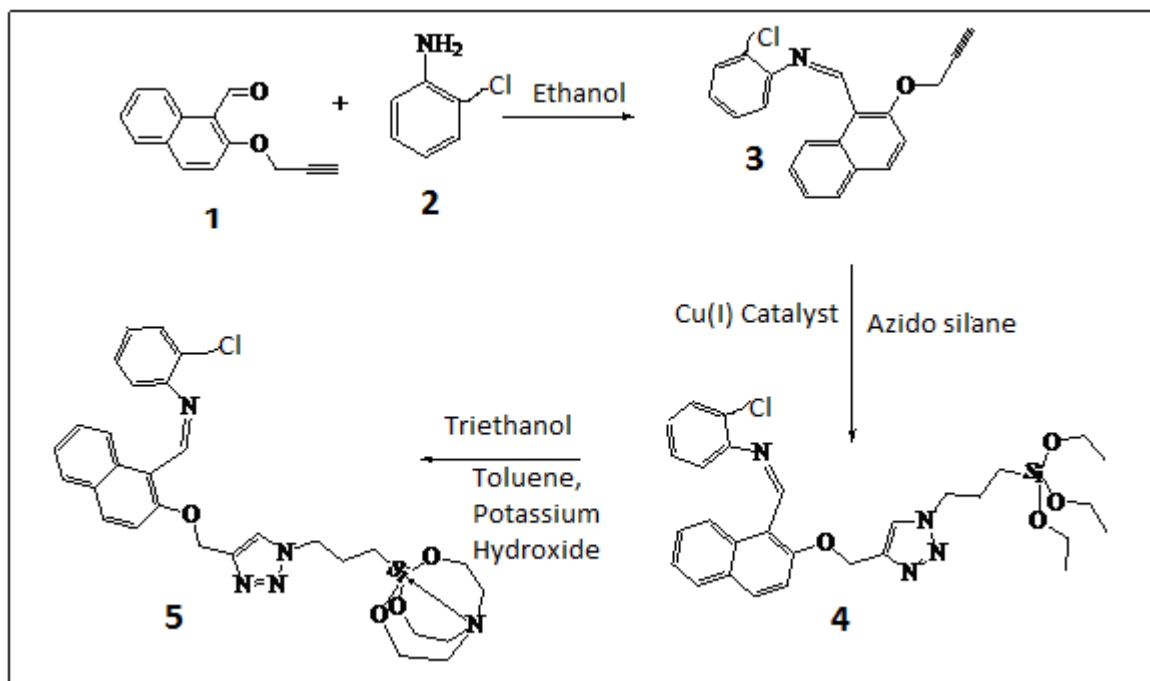
1. Introduction

The scientist Jeremy Musher was the first scientist in the world who had first of all discovered the terminology of hypervalent compounds [1]. This hypervalent concept was very very helpful in the explanation of various compounds of the especially main group member elements [2]. When a compound is hybridized mixed with the nitrogen hetero cycle then it opens a very wide era in the different fields on the globe for their specific uses [3]. When hypervalent compound is silicon then it couples with the organic framework that is specially the heterocyclic triazole ring then it is very beneficial and useful [4]. This coupled framework of organosilicon are synthesized in such a way that it gives trialokxy silanes and silatranes which have the open a field of organometallic chemistry into new field having biological and chemo sensing specificity [5]. These trialokxy silanes and silatranes are very very important and they have been synthesized with the help of click chemistry reaction and with the help of transesterification reaction [6]. In the click chemistry reaction terminal alkyne and azide react with each other and give rise to triazole heterocycle ring but on the other hand in the transesterification reaction tripodal ligand is used with the trialokxy group [7-9]. At the end of this transesterification reaction silatranes are formed which have a hypervalent organo silicon atom is present having five bonds at the silicon centre [10]. On the exocyclic position of this hypervalent silicon organic framework is present which is basically expand the properties of organo silicon compounds [11].

2. Experimental Part

All the compounds which have been used are taken from the reputed company that is from the AVRA. They are used as they are received from the employer. Rest all the synthesis have been carried out under inert atmosphere because the silanes and silatranes are hygroscopic in nature and they get easily affected by the presence of air and moisture.

2.1 Synthesis of silatrane 5 that is N-((2-((1-(3-(2,8,9-trioxa-5-aza-1-sila-bicyclo [3.3.3]undecan-1-yl) propyl)-1H-1,2,3-triazol-4-yl) methoxy) naphthalen-1-yl) methylene)-2-chloro benzenamine. This compound is already synthesized in the literature according to the reported literature [12]. In the synthetic procedure of this compound 5 first of all 2-chlorobenzeneamine is taken which is further very easily coupled with the hypercoordinated organo silicon atom via two different procedure stepwise. By using this methodology commercially 2-chlorobenzeneamine which was available was coupled with the Schiff base compound that is with the compound 3 which was further converted into the terminal alkyne which have special group that is Schiff base was present. This terminal alkyne having a Schiff base structure was used in the cycloaddition step with the azido silane as shown in the scheme as given below. This step is only possible with help of Cu(I) Catalyst (Scheme 1). The newly synthesized compound 4 that means cyclized silane product was successfully and quantitatively converted into the target molecule that is compound 5. In the compound 5 that is in the silatrane hypervalent silicon atom was present having five bonds and tricyclic ring. In addition to this compound 5 has triazole connector present at the centre which connect the tricyclic part with organic framework having Schiff base sub unit at the second terminal. The silatranes are formed via a well known reaction that is transesterification reaction (which is also called as transesterification reaction) in dry toluene solvent. These compounds are synthesized in a very purified manner and their purity was cross-checked by the elemental analysis technique, melting point, and IR technique and NMR spectroscopic technique. It might be mentioned here that these techniques were reasonably good to check the purity and identification of the compounds.



Scheme : Synthesis of Silatrane Triazole, silane and hypervalent silatrane compounds.

3. Result and Discussion Part

3.1 IR studies

The IR spectroscopic studies gave a very efficient and significant evidences that all these compounds had been formed or synthesized successfully. The IR was taken and recorded in a very efficient way in the range of $4000\text{--}400\text{ cm}^{-1}$. In the spectra it was observed that there is a very clear and region around the 2100 cm^{-1} which gives the 100% confirmation of the authentication of cyclization of azido silane with the terminal alkyne having Schiff base which produce compound 4 that is cyclized silane having triazole bridged that is compound 4 as shown in the scheme above. In addition to this the absorption bands around 2877 cm^{-1} and 1678 cm^{-1} which correlates the presence of aromatic Schiff base and presence of one more sub unit that is presence of triazole ring. Also transannulane bond which was the fifth bond formed from Nitrogen atom to Si atom as dative bond N–Si in the silatrane 5 was confirmed presence of absorption band at the 678 cm^{-1} .

3.2 NMR studies

The NMR studies had been carried out of all the above synthesized compounds. ^1H NMR spectra of triethoxysilane 4 which have Schiff base, triazole ring and three ethoxy groups were attached in the single molecule have been shown that in compound 5, three set of multiplets which were because of the --CH_2 units of propyl at δ 1.90 ppm. In addition to this --OCH_2 which is actually joined with the clamped triazole ring was de-shielded and it was appeared at δ 5.33 ppm. From all these aside only aromatic ring protons which were just

neighbors of the Schiff base are confirmed by the appearance of multiplet signals in the range of δ 7.21– 7.28 ppm. The $-\text{CH}=\text{N}$ group proton was present around the range of 8.10 ppm. Moreover, the protons which were present as $-\text{OCH}_2\text{CN}$ protons in the silatranes rings gives the triplet peaks at δ 3.44–3.66 ppm. He considerable change of silatrane NMR from that of silatrane NMR is basically totally disappearance or missed peaks at δ 3.86–3.6 ppm and δ 1.22–1.11 ppm and new two peaks were formed at δ 3.61 which is due to $-\text{NCH}_2\text{CH}_2\text{O}-$ and 2nd peak at δ 2.77 ppm which was basically because of $-\text{NCH}_2\text{CH}_2\text{O}-$ protons in arms of atrane ring.

The NMR spectra when recorded for C-13 then in the ^{13}C NMR spectra, the specific the considerable downfield shift was appeared in the spectra which was of group of $-\text{N}_3\text{C}-$ of triazole and it displaces from the δ 60.2–54.3 ppm to of δ 132.2–126.8 ppm. The methylene carbon of the propyl chain which was directly joined to the silicon atom and it appears at δ = 8.9 ppm for triethoxysilanes and but in case of the silatrane molecule which have hypervalent carbon atom then this group was appeared at the δ = 14.2 ppm for silatranes. This shift of methylene in the direction of downfield region gives the clear indication of presence of that carbon atom which was joined to the hypervalent silicon atom. Also in addition to these peaks, peaks due to $\text{CH}_2\text{CH}_2\text{N}_3$ group was appeared at the δ = 25.7 ppm and δ = 54.4 ppm, respectively. The ethoxy group in the cyclized silane was confirmed by two peaks at the δ = 58.4 ppm and δ = 18.8 ppm.

3.3 Antibacterial assay

Here in this study all the synthesized complex molecules are studied for their antibacterial activity. They were tested in relation to their specific property that means for their anti-bacterial action against gram positive and gram negative bacteria. The gram negative bacteria which were used in this experiment are *Klebsiellapneumoniae*, *P. aeruginosa*, and used gram positive bacteria are *S. aureus* and *S. epidermidis*. This experiment was done with the help of well plate assay and these compounds gave best effective results against these taken bacteria found. From all these synthesized compounds, the compound 5 having MIC of 19.7 $\mu\text{g}/\text{ml}$ was the superior effective agent against *P. aeruginosa* from these four bacteria. This compound 5 gave the more efficient and best result than the already medicine Cefepime which is available in the market today.

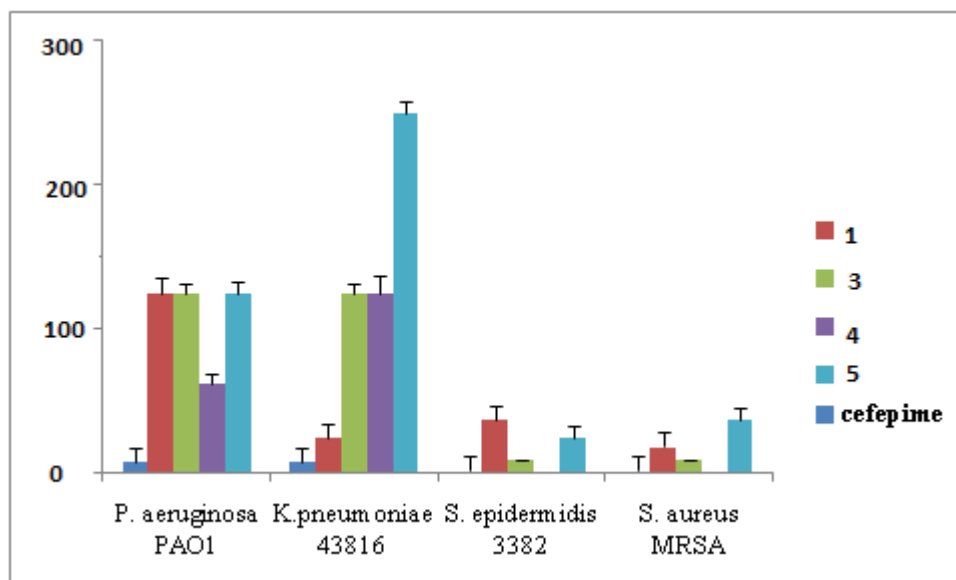
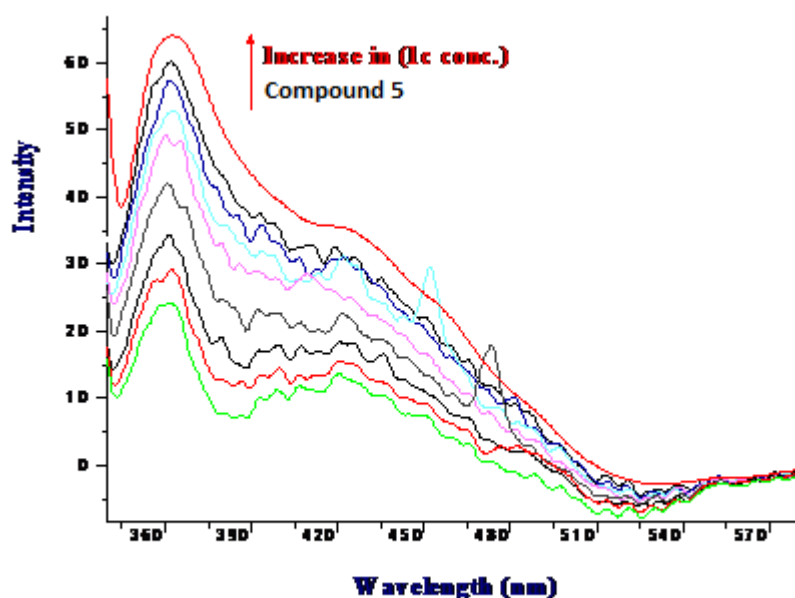
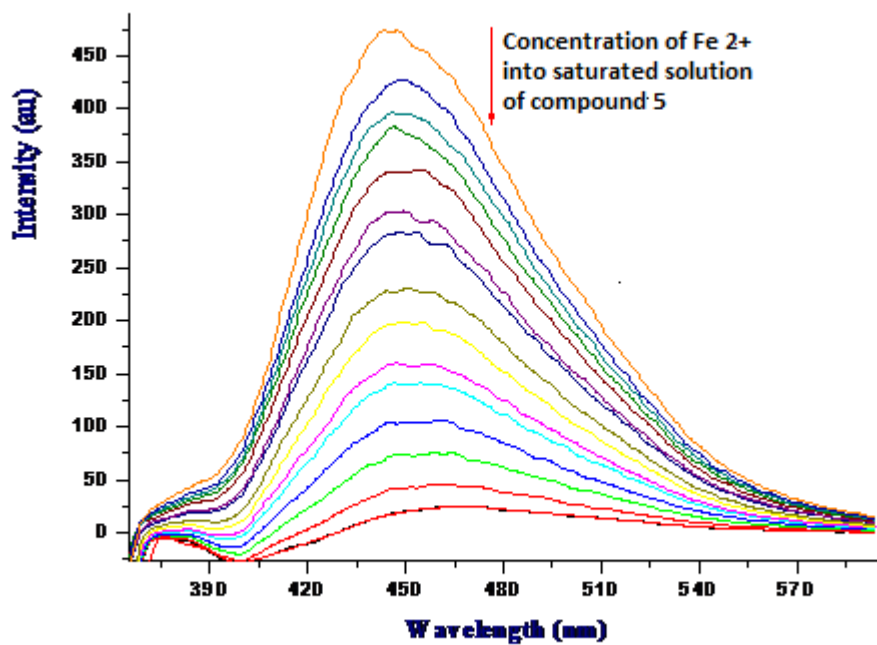


Figure 1: The relative MIC of four compounds 1-5 and Cefepime

3.4 Chemo sensing activity

The compound 5 was used for this testing of number of cations. Only compound 5 was used because it was the most stable compound among silanes and silatranes as well as it was the hypervalent organo silicon compound which attract the attention of researchers. By the testing on the Infra Red Spectrophotometer it was observed that only the Fe^{2+} cation is sensed by this compound. As we added the Fe^{2+} cationic solution into the saturated solution of compound of 5 in the methanol solvent then the peak intensity become decreases as we added more and more





Fe^{2+} cation concentration. This is because due to addition of Fe^{2+} cations, the Fe^{2+} cations binds with the compound 5 and gave rise to a metal framework complex in which Fe^{2+} cations were being captured.

4. Conclusion

Compound 5 acts as a efficient chelating agent or framework to capture the the specific Fe^{2+} ion from many metal ions as they were tested. These all compounds were successfully synthesized and characterized by many spectroscopic techniques. In addition to this these compounds are also act as anti bacterial agent and best anti bacterial activity is shown by the compound 5 from all the newly synthesized compounds. So in future they will definitely replace the traditional drugs as well as many Fe^{2+} chemo sensors.

5. References

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