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# The Possibility of Silicon-Based Life

**Ricardo Gobato[1], Alireza Heidari[2,*], Abhijit Mitra[3],Lauro Figueroa Valverde[4]**

**Authors' Affiliations**
[1] Green Land Landscaping and Gardening, Seedling Growth Laboratory, 86130-000, Parana, Brazil.
[2] Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA.
[3] Department of Marine Science, University of Calcutta, 35 B.C. Road Kolkata, 700019, India.
[4]University Autonomous of Campeche (Faculty of Chemical-Biological Sciences), Calle Av. AgustínMelgar s/n, Buenavista, 24039 Campeche, Mexico.

***Corresponding Author**
**Alireza Heidari,** Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA.
**E-mails:** Scholar.Researcher.Scientist@gmail.com; Alireza.Heidari@calsu.us

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**ABSTRACT**

Silicon is the most obvious potential substitute for carbon, and the Possibility of Silicon-Based Life is the focus of the work. An analysis of the sites of action of four silicon-based exobiological nanomolecules, determined by the distribution of electrical charges around the nanomolecules atoms called: ASi, CSi, GSi and TSi. The Van der Waals radius distribution calculations have been determined via *ab initio* Hartree-Fock methods, Unrestricted and Restrict (UHF and RHF) in the set of bases used Effective Core Potential (ECP) minimal basis, and CC-pVTZ (Correlation-consistent valence-only basis sets triple-zeta). Polymers can also be assembled as chains of alternating elements such as Si-C, Si-O, and B-N. Alternation with carbon is used to some extent in terran organisms (such as C-C-N in proteins and C-C-C-O-P-O in nucleic acids), and silated compounds play important structural roles in the cells of many organisms on Earth.

**Keywords**: Silicon, Astrobiology, Exobiology, Hartree-Fock Methods, Van der Waals, Life

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## 1. INTRODUCTION

On the basis in chemical evolutionary theory, it is implicit that life is being based upon carbon chemistry. [1] The possibility of life based on silicon has been discussed extensively (though casually). Theoretical chemical arguments have been proposed to support this presumption. [1]

The most significant result would be to and some type of living matter radically different from that of the Earth. One might cite under this category supposed organisms with a structure and metabolic machinery based on silicon rather than on carbon; or forms with an ammonia based rather than a water based machinery and metabolism. (One should note in the former case, however, that fully aerobic silicon metabolizers would be required to exhale quartz.) [1]

Exclude the noble gases from consideration because of their inertness; the four most abundant elements of the universe are hydrogen, oxygen, carbon, and nitrogen. In fact, hydrogen is the major constituent of the universe; oxygen, carbon, and nitrogen are each about ten times more plentiful than the next most abundant element, silicon. [1]

In comparing the carbon and silicon has: the Si lies in the same column of the periodic table of the elements, and it has been investigated as a possible alternative for building up biological molecules in exobiology. [2,3]

The option for simple replacement of carbon by silicon [4,5] is due to the peculiar characteristics between both. Atomic interactions under non-carbon conditions were studied, with only the Hydrogen, Silicon, Nitrogen and Oxygen atoms, in STP (Standard Temperature and Pressure), for the four standard bases of DNA, A, C, G and T, thus obtaining by quantum chemistry four new compounds, named here as: ASi, CSi, GSi and TSi. [6, 7], [8, 9], [10, 11]

Silicon based chemistry, however, is by far less flexible than carbon chemistry, not able to form double covalent bonds with the same easiness as Carbon does. Other fact is the larger volume occupied by the external electronic orbitals of silicon tend to reduce the superposition of *p* orbitals. [2, 3]

Through the chemical abundances of biological elements in the earth crust, terrestrial life has chosen carbon instead of silicon, in spite of the larger abundance of silicon. This fact suggests that carbon is better suited to form biological molecules. [2, 3]

However, this paper assumes conditions without the presence of Carbon.Calculations obtained in the *ab initio* Unrestricted and Restrict Hartree-Fock method, (UHF and RHF). The set of basis used Effective core potential (ECP) minimal basis, CC-pVTZ (Correlation-consistent valence-only basis sets triple-zeta). [12, 13], [14, 15], [16, 17], [18]

## 2. THE POSSIBILITY OF SILICON-BASED LIFE

Silicon is the most obvious potential substitute for carbon. It is also a *p*-block element of group IV, just below carbon in the periodic table. With four electrons in its outer shell, it has somewhat similar physical properties to carbon. Silicon and carbon are both small elements with small atomic weights and small atomic numbers, with carbon being the smaller of the two. Both elements have very high melting and boiling points, with carbon having the higher of the two. Both elements are in the mid-range of electronegativity's, but again carbon is higher. Both are solids at standard temperatures and pressures (STP) (298 K, 105 Pa) and both are semi-metallic. They both form sp3 hybrid orbitals with tetrahedral structures in many of their compounds. [19]

Silicon has a larger radius and therefore forms relatively weak bonds with the light elements that are abundant in the universe. The electrons in carbon are closer to the nucleus, and thus form stronger bonds that can retain light elements much better. This increases carbon's chance of forming complex compounds. The Si-Si bond strength is lower than the C-C bond strength, thus carbon is much more likely to bond with itself than silicon. The smaller Si-Si bond energy is also reflected in silicon's lower energy of vaporization. Silicon rarely forms any double or triple bonds, but double bonds and triple bonds are common and of great biological significance for carbon. [19]

Carbon exhibits many characteristics that make it uniquely suited for life- supporting processes. Its usefulness for life derives primarily from

1. the versatility that enables it to form millions of complex polymers, including single, double and triple bonded compounds, chiral compounds, and resonant ring structures;
2. the ease with which it changes from one valence state to another, thereby suiting it well for energy-transferring redox reactions; and
3. its compatibility with water (and ammonia) as a liquid solvent.
   The only other element that approaches the versatility of carbon and is common enough to be a universal building block is silicon. Silicon can form long chains as silanes, silicones, and silicates.

Some of these compounds could present a possible alternative to carbon for the construction of polymers under very restricted environmental conditions. These are:

1. little or no oxygen;
2. little or no liquid water;

3. temperatures above 493 K (silicones, silicates) or below 273 K (silanes);
4. pressures greater than on the surface of Earth;
5. presence of a solvent such as methane or methanol; and
6. relative lack of available carbon.

Other elements would likely not be suitable as backbones for the building blocks of a living system. However, it is not clear that polymeric skeletons have to be built from one element only. Polymers can also be assembled as chains of alternating elements such as Si-C, Si-O, and B-N. Alternation with carbon is used to some extent in terran organisms (such as C-C-N in proteins and C-C-C-O- P-O in nucleic acids), and silated compounds play important structural roles in the cells of many organisms on Earth. But no comprehensive bioenergetic metabolism is known to arise from non-carbon complex chemistry, despite the high abundance of oxygen and silicon on Earth, and the relative concentration of silicon on other terrestrial planets. Thus, if elements other than carbon constitute the building blocks for any living system on other worlds, they almost surely exist under conditions far different from those on Earth, including temperatures and pressures where water could not be the solvent. Titan provides the best natural laboratory in our Solar System for investigating this possibility. [19][20, 21], [22, 23], [24, 25], [26, 27], [28, 29], [30, 31].

## 3. HARTREE-FOCK METHODS, HARDWARE AND SOFTWARE

For calculations the computer used for was a Desktop with SUSE Linux Enterprise Desktop [19], AMD Ryzen 7 1800X processor [32], ASUS [33] Prime A320M-K motherboard, 16GB of RAM, with 500GB SSD. [34]

The *ab initio* [12,13], [14,15], [16,17], [18] calculations have been per- formed to study the equilibrium configuration, and calculation of the Mulliken [12] loads for CC-pVTZ [12] exobiological molecules of the study. The set of programs GaussView 5.0.8 [35], GAMESS, BIOVIA Draw 2017 [36], and CHARMM22 [37, 38] were used.

## 4. RESULTS AND MOLECULES PROPERTIES

The distribution of leptons in ASi, CSi, GSi and TSi molecules, were obtained through computationally calculated using the *ab initio* Hartree-Fock (HF) method. [6,7], [8, 9], [10,11] The Figures (1-4) show the distribution of Mulliken electrical charges around the atoms of exobiological molecules, using a scale of 0.75 of the Van der Waals radius. With a color gradient going from red, black to green, that is, gradient of negative charges in red, to green, positive charges, respectively.

### 4.1 ASi

IUPAC name:
2,3,4,5,6,7,8,9-octahydro-1H-[1,3,2,4,5]diazatrisilolo[4,5-d][1,3,2,4,5,6]diazatetrasilin-8-amine; [6, 7], [8, 9], [10, 36]
E (RHF): -1719.94065566 a. u.; [17, 18]
Dipole Moment: 3.2363 Debye; [17, 18]
Molecular Formula: $H_{13}N_5Si_5$.

Nitrogen and Silicon atoms present strong bonding potentials, prone to Hydrogen bonds, due to the shifts of charges of Silicon atoms (cationic), while Nitrogens (anionic). With the exception of Silicon from the central ring bonded to Nitrogen and other Silicon.

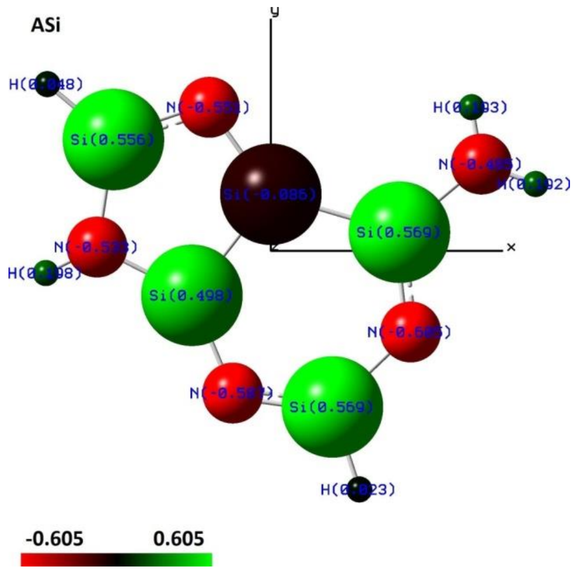


**Figure 1**: Representation of the molecular structure of ASi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 [35].

**4.2 CSi**
IUPAC name:
2-hydroxy-1,3,2,4,5,6-diazatetrasilinan-4-amine; [6, 7], [8, 9], [10, 36]
E (UHF): -1396.96978499 a. u.; [17, 18]
Dipole Moment: 10.6516 Debye; [17, 18]
Molecular Formula: $H_{11}N_3OSi_4$.

Oxygen and Nitrogen are anionic and two Silicon atoms (cationic), thus concentrating on these hydrogen bonds.

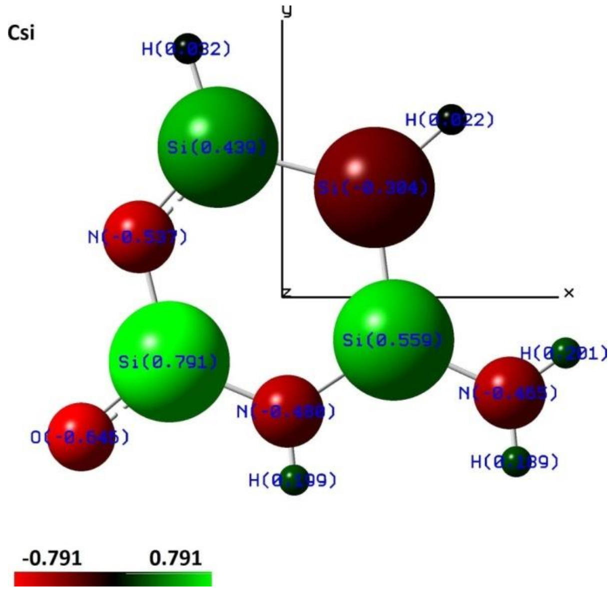


**Figure 2**: Representation of the molecular structure of CSi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 [35].

**4.3 GSi**
IUPAC name:
8-oxo-3,7-dihydro-[1,3,2,4,5]diazatrisilolo[4,5-d][1,3,2,4,5,6]diazatetrasilin-6-amine; [6, 7], [8, 9], [10, 36]
E (RHF): -1791.74221629 a. u.; [17, 18]
Dipole Moment: 9.7172 Debye; [17, 18]
Molecular Formula: $H_5N_5OSi_5$.

GSi has the highest dipole moment due to the displacement of electrical charges between the atoms of the molecule.

The Oxygen atom is anionic, while three Silicon atoms are cationic, and one anionic. These have strong potential for forming hydrogen bonds.

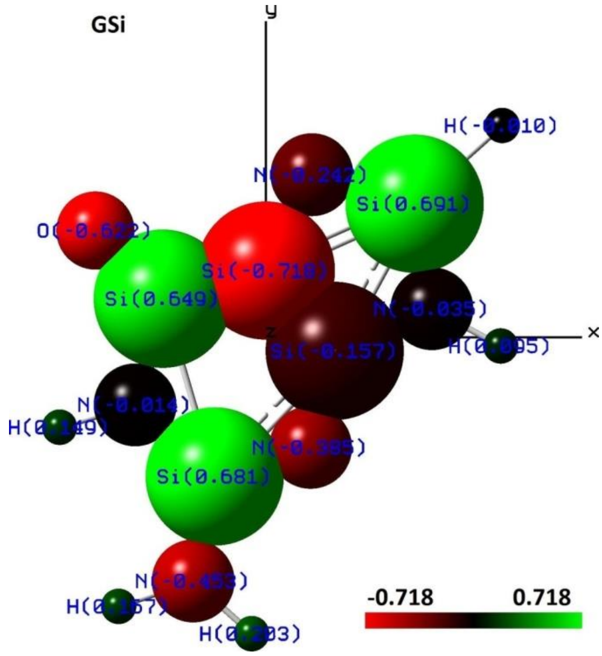


**Figure 3**: Representation of the molecular structure of GSi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 [35].

**4.4 TSi**

IUPAC name:
(2,4-dihydroxy-1,3,2,4,5,6-diazatetrasilinan-5-yl)silane; [6, 7], [8, 9], [10, 36]
E (RHF): -1706.93799137 a. u.; [17, 18]
Dipole Moment: 8.7051 Debye; [17, 18]
Molecular Formula: $H_{12}N_2O_2Si_5$.

The two oxygen atoms as well as the two nitrogen atoms are anionic as expected, due to the displacement of charges from the predominantly cationic silicons.

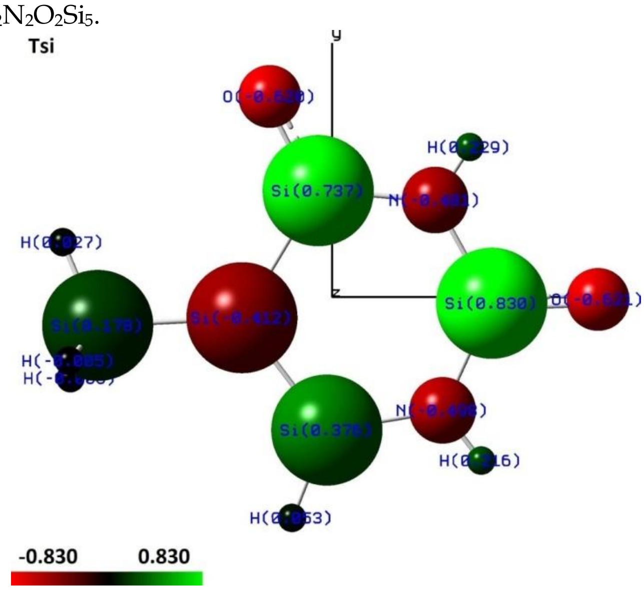


**Figure 4**: Representation of the molecular structure of TSi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 [35].

## 5. CONCLUSIONS

Dipole moment of nanomolecules in decreasing order: CSi > GSi > TSi > ASi;
The Energy E (HF): GSi > CSi > ASi > TSi; and Mulliken Charge Range: TSi > CSi > GSi > ASi.

The study has so far been limited to computational *ab initio* methods. The results are compatible with the theory of quantum chemistry, but their proof experimental verification depend on advanced techniques for their synthesis, obtaining in laboratory for experimental biochemical.

If elements other than carbon constitute the building blocks for any living system on other worlds, they almost surely exist under conditions far different from those on Earth, including temperatures and pressures where water could not be the solvent. [19]

Titan provides the best natural laboratory in our Solar System for investigating this possibility. [19]

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