The Possibility of Silicon-Based Life

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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 basis 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

1 Introduction

On the basis in chemical evolutionary theory, it is implicit that life is being based upon carbon chemistry. Mamikunian and (Eds.), 1965

The possibility of life based on silicon has been discussed extensively (though casually). Theoretical chemical arguments have been proposed to support this presumption. Mamikunian and (Eds.), 1965

The most significant result would be to find 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.) Mamikunian and (Eds.), 1965

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. Mamikunian and (Eds.), 1965

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. Shaw, 2006; Horneck and Rettberg, 2007

The option for simple replacement of carbon by silicon McDouall, 2013; Patai and Rappoport, 1989 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. Gobato, 2021; Gobato et al., 2021,Gobato et al., n.d.(a); Gobato et al., n.d.(b),Gobato et al., n.d.(c); Gobato et al., n.d.(d)

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. Shaw, 2006; Horneck and Rettberg, 2007

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. Shaw, 2006; Horneck and Rettberg, 2007

However, this paper assumes conditions without the presence of Carbon.

Calculations obtained in the ab initio Unrestricted and Restrict Hartree-Fockmethod, (UHF and RHF). The set of basis used Effective core potential (ECP) minimal basis, CC-pVTZ (Correlation-consistent valence-only basis sets triple-zeta). Levine, 2003; Kohn and Sham, n.d.,Thijssen, 2001; Wilson, Mourik, and Jr., 1996,"Computational Methods in Optimization" 1971; Gordon and Schmidt, 2005,Gordon, 1993

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 electronegativities, 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 sp^3 hybrid orbitals with tetrahedral structures in many of their compounds. Dirk Schulze-Makuch, 2008

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.Dirk Schulze-Makuch, 2008

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 triplebonded 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. (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. Dirk Schulze-Makuch, 2008 Muriel Gargaud, 2006; John Barrow, 2008,Joseph Seckbach (auth.), 2005; Julian Chela-Flores (auth.), 1998,M, 2006; Agency, 1999,Gerda Horneck, 2007; William Sallun Filho, 2011,Brandner W., 2006; Barrow J., 2008,Muriel Gargaud, 2005; (Author), 2006.

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 Enc, 2022b, ASUS Enc, 2022a Prime A320M-K motherboard, 16GB of RAM, with 500GB SSD. 2022

The *ab initio* Levine, 2003; Kohn and Sham, n.d.,Thijssen, 2001; Wilson, Mourik, and Jr., 1996,"Computational Methods in Optimization" 1971; Gordon and Schmidt, 2005,Gordon, 1993 calculations have been performed to study the equilibrium configuration, and calculation of the Mulliken Levine, 2003 loads for CC-pVTZ Levine, 2003 exobiological molecules of the study. The set of programs GaussView 5.0.8 Dennington, Keith, and Millam, 2009, GAMESS[1], BIOVIA Draw 2017 "Computational results obtained using software programs from Dassault Systèmes BIOVIA. The ab initio calculations were performed with the DMol3 program, and graphical displays generated with Draw" 2017, and CHARMM22 Brooks et al., 1983; Brooks et al., 2009 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. Gobato, 2021; Gobato et al., 2021,Gobato et al., n.d.(a); Gobato et al., n.d.(b),Gobato et al., n.d.(c); Gobato et al., n.d.(d)

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.

[1]Computational chemistry software program and stands for General Atomic and Molecular Electronic Structure System (GAMESS) Gordon and Schmidt, 2005; Gordon, 1993

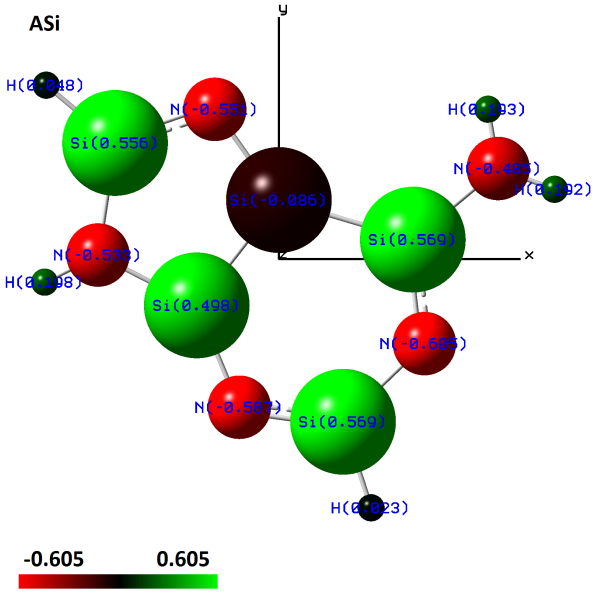

Figure 1: *Representation of the molecular structure of ASi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 Dennington, Keith, and Millam, 2009.*

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; Gobato, 2021; Gobato et al., 2021,Gobato et al., n.d.(a); Gobato et al., n.d.(b),Gobato et al., n.d.(c); "Computational results obtained using software programs from Dassault Systèmes BIOVIA. The ab initio calculations were performed with the DMol3 program, and graphical displays generated with Draw" 2017
E(RHF): -1719.94065566 a. u.; Gordon and Schmidt, 2005; Gordon, 1993
Dipole Moment: 3.2363 Debye; Gordon and Schmidt, 2005; Gordon, 1993
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.

4.2 CSi

IUPAC name:
2-hydroxy-1,3,2,4,5,6-diazatetrasilinan-4-amine; Gobato, 2021; Gobato et al., 2021,Gobato et al., n.d.(a); Gobato et al., n.d.(b),Gobato et al., n.d.(c); "Computational results obtained using software programs from Dassault Systèmes BIOVIA. The ab

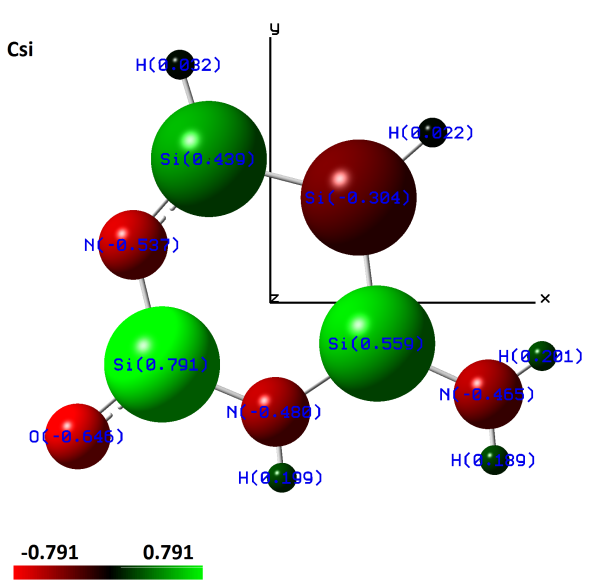

Figure 2: *Representation of the molecular structure of CSi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 Dennington, Keith, and Millam, 2009.*

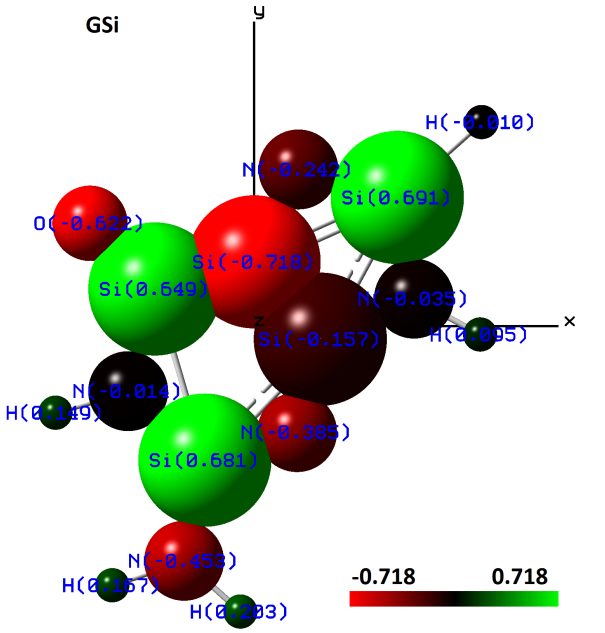

Figure 3: *Representation of the molecular structure of GSi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 Dennington, Keith, and Millam, 2009.*

initio calculations were performed with the DMol3 program, and graphical displays generated with Draw" 2017
E(UHF): -1396.96978499 a. u.; Gordon and Schmidt, 2005; Gordon, 1993
DipoleMoment: 10.6516 Debye; Gordon and Schmidt, 2005; Gordon, 1993
Molecular Formula: $H_{11}N_3OSi_4$.

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

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; Gobato, 2021; Gobato et al., 2021,Gobato et al., n.d.(a); Gobato et al., n.d.(b),Gobato et al., n.d.(c); "Computational results obtained using software programs from Dassault Systèmes BIOVIA. The ab initio calculations were performed with the DMol3 program, and graphical displays generated with Draw" 2017
E(RHF): -1791.74221629 a. u.; Gordon and Schmidt, 2005; Gordon, 1993
Dipole Moment: 9.7172 Debye; Gordon and Schmidt, 2005; Gordon, 1993
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.

4.4 TSi

IUPAC name:
(2,4-dihydroxy-1,3,2,4,5,6-diazatetrasilinan-5-yl)silane; Gobato, 2021; Gobato et al., 2021,Gobato et al., n.d.(a); Gobato et al., n.d.(b),Gobato et al., n.d.(c); "Computational results obtained using software programs from Dassault Systèmes BIOVIA. The ab initio calculations were performed with the DMol3 program, and graphical displays generated with Draw" 2017
E(RHF): -1706.93799137 a. u.; Gordon and Schmidt, 2005; Gordon, 1993
DipoleMoment: 8.7051 Debye; Gordon and Schmidt, 2005; Gordon, 1993
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.

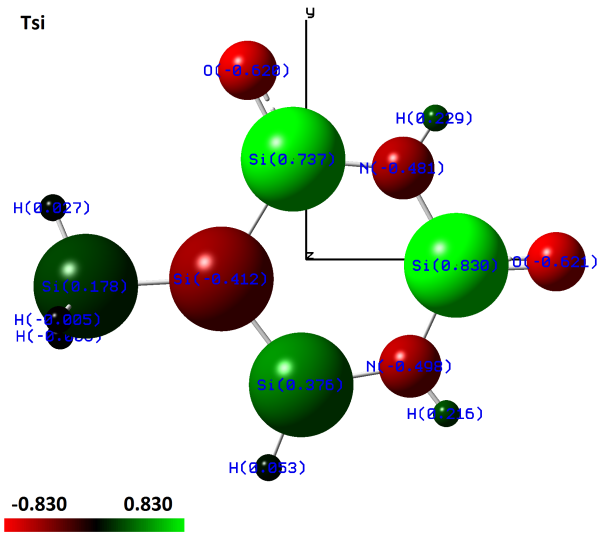

Figure 4: *Representation of the molecular structure of TSi molecule with distribution of Mulliken electrical charges. Images obtained in the software Gaussview, Version 5, 2009 Dennington, Keith, and Millam, 2009.*

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 comprovation 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. Dirk Schulze-Makuch, 2008

Titan provides the best natural laboratory in our Solar System for investigating this possibility. Dirk Schulze-Makuch, 2008

References

(2022). In: *Creative Commons. (CC-BY 4.0)*.

Agency, A Brack; B Fitton; F Raulin; A Wilson; European Space (1999). *Exobiology in the solar system and the search for life on Mars : report from the ESA Exobiology Team Study, 1997-1998*. ESA SP, 1231. ESA Publications Division. ISBN: 9290925205,9789290925200. URL: http://gen.lib.rus.ec/book/index.php?md5=26de47d64f2a223c93e79f91276c0565.

(Author), Andrew M. Shaw (2006). *Astrochemistry: From Astronomy to Astrobiology*. 1st ed. ISBN: 9780470091371,0470091371,0470091363,9780470091364,978 URL: http://gen.lib.rus.ec/book/index.php?md5=1a6cb0994a26712aadd2d316dfd0bb2d.

Barrow J. Morris S.C., Freeland S. Harper C. (eds.) (2008). *Fitness of the cosmos for life*. Cambridge Astrobiology. CUP. ISBN: 0521871026,9780521871020. URL: http://gen.lib.rus.ec/book/index.php?md5=eac0a8d1ba38973baf071e3cee69c263.

Brandner W., Klahr H. (eds.) (2006). *Planet formation*. Cambridge Astrobiology. CUP. ISBN: 0521860156,9780521860154. URL: http://gen.lib.rus.ec/book/index.php?md5=6a49362b78ec541f3e9e1f00cd9ec988.

Brooks, B. R. et al. (2009). "CHARMM: A Program for Macromolecular Energy, Minimization, and Dynamics Calculations". In: *J. Comp. Chem* 30, pp. 1545–1614.

Brooks, R. et al. (1983). "CHARMM: A Program for Macromolecular Energy, Minimization, and Dynamics Calculations". In: *J. Comp. Chem* 4, pp. 187–217.

"Computational Methods in Optimization" (1971). In: *Elsevier* 77.

"Computational results obtained using software programs from Dassault Systèmes BIOVIA. The ab initio calculations were performed with the DMol3 program, and graphical displays generated with Draw" (2017). In: *BIOVIA Draw 2017 Enterprise. MDL Draw Editor 17.1.0.900*.

Dennington, R., T. Keith, and J. Millam (2009). "Gaussview, Version 5". In.

Dirk Schulze-Makuch, Louis N. Irwin (2008). *Life in the Universe: Expectations and Constraints (Advances in Astrobiology and Biogeophysics)*. 2nd. Advances in Astrobiology and Biogeophysics. Springer. ISBN: 3540768165,9783540768166. URL: http://gen.lib.rus.ec/book/index.php?md5=c9a17a2a0774c5c652be8ffda7b968a1.

Enc, Wikipedia. The Free (2022a). "Asus". In: *Creative Commons. (CC-BY 4.0)*.

– (2022b). "Ryzen". In: *Creative Commons. (CC-BY 4.0)*.

Gerda Horneck, Petra Rettberg (2007). *Complete Course in Astrobiology*. Wiley-VCH. Physics Textbook. Wiley-VCH. ISBN: 3527406603,9783527406609. URL: http://gen.lib.rus.ec/book/index.php?md5=49b09e86a887d86558c17faf259dfdd0.

Gobato, R. (2021). "Infrared Spectrum for the New Nanomolecules ASi, CSi, TSi and GSi". In: *Arch Biomed Eng and Biotechnol* 5, p. 3.

Gobato, R. et al. (n.d.[a]). “Applying Ab Initio Hartree-Fock Methods to Exobiology Nano-Molecules”. In: *ResearchGate* (). URL: 10.13140/RG.2.2.31901.44004.

– (n.d.[b]). “Applying Ab Initio Hartree-Fock Methods to Exobiology Nano-Molecules”. In: *J Current Eng Techno* 3 ().

– (n.d.[c]). “Infrared Spectrum for the New Exobiological Nanomolecules Asi, Csi, Tsi and Gsi”. In: *Sumerianz Journal of Scientific Research* 4 ().

Gobato, R. et al. (n.d.[d]). “Spectroscopy and Dipole Moment of the Molecule C13H20BeLi2SeSi via Quantum Chemistry Using Ab Initio, Hartree–Fock Method in the Base Set CC–pVTZ and 6–311G**(3df, 3pd)”. In: *American Journal of Quantum Chemistry and Molecular Spectroscopy* 2 ().

Gobato, R. et al. (2021). “Applying, "Ab Initio" Hartree-Fock Methods to Exobiological Nanomolecules”. In: *Physics of Biology*. URL: vixra.org/abs/2104.0091.

Gordon, M. S. and M. W. Schmidt (2005). “Advances in electronic structure theory: GAMESS a decade later. Theory and Applications of Computational Chemistry: the first forty years”. In: *Elsevier. C. E. Dykstra, G. Frenking, K. S. Kim and G.E.Scuseria (editors)*, 1167–1189.

Gordon, M. S. et al. (1993). “General atomic and molecular electronic structure system (GAMESS)”. In: *J. Comput. Chem* 14, 1347–1363.

Horneck, G. and P. Rettberg (2007). *Complete Course in Astrobiology*. Series: Physics Textbook, Wiley-VCH.

John Barrow Simon Conway Morris, Stephen Freeland Charles Harper (2008). *Fitness of the cosmos for life: biochemistry and fine-tuning*. 1st ed. Cambridge astrobiology 2. Cambridge University Press. ISBN: 0521871026,9780521871020,9780511371080. URL: http://gen.lib.rus.ec/book/index.php?md5=93bd1e56297fd8e9830aa31a3f06d70a.

Joseph Seckbach (auth.), Joseph Seckbach (eds.) (2005). *Origins: Genesis, Evolution and Diversity of Life*. 1st ed. Cellular Origin, Life in Extreme Habitats and Astrobiology 6. Springer Netherlands. ISBN: 978-1-4020-1813-8,978-1-4020-2522-8. URL: http://gen.lib.rus.ec/book/index.php?md5=214101b50f3bb3a05c4d93408ce634a1.

Julian Chela-Flores (auth.) Julian Chela-Flores, François Raulin (eds.) (1998). *Exobiology: Matter, Energy, and Information in the Origin and Evolution of Life in the Universe: Proceedings of the Fifth Trieste Conference on Chemical Evolution: An Abdus Salam Memorial Trieste, Italy, 22–26 September 1997*. 1st ed. Springer Netherlands. ISBN: 978-94-010-6124-7,978-94-011-5056-9. URL: http://gen.lib.rus.ec/book/index.php?md5=771afe870f959dc7423d64249db3efa6.

Kohn, W. and L. J. Sham (n.d.). “Self-consistent equations including exchange and correlation effects”. In: *Phys. Rev* 140 ().

Levine, I. N. (2003). *Quantum Chemistry*. Pearson Education (Singapore) Pte.Ltd., Indian Branch, 482 F. I. E. Patparganj, Delhi 110 092, India, 5th ed. edition.

M, Shaw A (2006). *Astrochemistry[c] From Astronomy to Astrobiology*. URL: http://gen.lib.rus.ec/book/index.php?md5=e04593c083f7b07a17fbda97e72ce757.

Mamikunian, G. and M. H. Briggs (Eds.) (1965). *Current Aspects of Exobiology*. Jet Propulsion Laboratory, California Institute of Technology.

McDouall, J. J. W. (2013). *Computational Quantum Chemistry. Molecular Structure and Properties in Silico*. The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 0WF, UK.

Muriel Gargaud Bernard Barbier, Hervé Martin Jacques Reisse C. de Duve (2005). *Lectures in Astrobiology: Vol I (Advances in Astrobiology and Biogeophysics)*. 1st ed. Springer. ISBN: 3540223150,9783540223153,3540290052,9783540290056. URL: http://gen.lib.rus.ec/book/index.php?md5=0150be28edcf59ce427df3be3d7cabaa.

Muriel Gargaud, Muriel Gargaud;HervÃ© Martin;Philippe Claeys (2006). *Lectures in astrobiology II*. 1st ed. Advances in Astrobiology and Biogeophysics. Springer. ISBN: 9783540336921,3-540-33692-3,3540336923. URL: http://gen.lib.rus.ec/book/index.php?md5=b162df1816decd533fa9f1b6db4df5fc.

Patai, S. and Z. Rappoport (1989). *The Chemistry of Organic Silicon Compounds*. Series: The Chemistry of functional groups, Wiley.

Shaw, A. M. (2006). *Astrochemistry: From Astronomy to Astrobiology*. ISBN: 9780470091364, 0470091363.

Thijssen, J. M. (2001). *Computational Physics*. Cambridge University Press, Cambridge.

William Sallun Filho Thomas Rich Fairchild (auth.), Vinod Tewari Joseph Seckbach (eds.) (2011). *Stromatolites: Interaction of Microbes with Sediments*. 1st ed. Cellular Origin, Life in Extreme Habitats and Astrobiology 18. Springer Netherlands. ISBN: 9400703961,9789400703964. URL: http://gen.lib.rus.ec/book/index.php?md5=24f95cabb893226a9d22a88d2a680043.

Wilson, A. K., T. van Mourik, and T. H. Dunning Jr. (1996). “Gaussian basis sets for use in Correlated Molecular Calculations. Sextuple zeta correlation consistent basis sets for boron through neon”. In: *J. Mol. Struct. (Theochem)* 388, 339–49.