



New Nano-Molecule Kurumi and Raman Spectroscopy using *ab initio*, Hartree-Fock Method

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Abstract

The work characterizes the Raman spectrum of the new nano-molecule $C_{13}H_{20}BeLi_2SeSi/C_{13}H_{19}BeLi_2SeSi$, nano-molecule Kurumi. Calculations obtained in the methods Restrict Hartree-Fock of the first principles (*ab initio*), on the set of basis used indicate that the simulated molecule $C_{13}H_{20}BeLi_2SeSi/C_{13}H_{19}BeLi_2SeSi$ features the structure polar-apolar-polar predominant. The set of basis used that have are correlation-consistent polarized Triple-zeta (CC-pVTZ) and Pople's basis sets six gaussian functions in the shell, three double zeta Gaussian functions, Slater type orbitals with polarization function (6-311G** (3df, 3pd)). In the CC-pVTZ base set, the charge density in relation to 6-311G** (3df, 3pd) is 50% lower. The length of the molecule $C_{13}H_{20}BeLi_2SeSi$ is of 15.799Å. The Raman spectrum was calculated indicating the characteristic of the nano-molecule and their frequency (cm⁻¹) were obtained in the set of bases used. The highest for Raman scattering activities peaks are in the frequency 3,348cm⁻¹ with 7.107609729 Å⁴/amu and 2,163 cm⁻¹ with 8.902805583 Å⁴/amu, for CC-pVTZ and 6-311G** (3df, 3pd), respectively. As the bio-inorganic molecule $C_{13}H_{20}BeLi_2SeSi$ is the basis for a new creation of a biomembrane, later calculations that challenge the current concepts of biomembrane should advance to such a purpose. The new nano-molecule Kurumi is well characterize computationally. As its scientific name 3-lithio-3-(6- {3-selena-8-beryllatricyclo [3.2.1.0^{2,4}] oct-6-en-2-yl} hexyl) -1-sila-2-lithacyclopropane.

Keywords: Biomembrane; CC-pVTZ ; Hartree-Fock method; Nano-molecule Kurumi; Raman spectroscopy; 6-311G** (3df, 3pd)

Introduction

The structure of the $C_{13}H_{20}BeLi_2SeSi$ is a bio-inorganic seed molecule for a biomembrane genesis that defies the current concepts of a protective mantle structure of a cell such as biomenbrane [1-3] to date is promising, challenging. Leaving to the Biochemists their experimental synthesis. Structures of a liquid crystal such as a new membrane may occur, micelles [1].

A large investigative study in the literature was carried out, but was not found of the structure studied here. There is an absence of a referential of the theme, finding only one work in [1]. The present study is an extension of the work already begun in the creation of *ab initio*, computational methods of quantum chemistry, to prove the possible structure of the bio-inorganic nano-molecule genesis, $C_{13}H_{20}BeLi_2SeSi$. Their characterization by well-known *ab initio* methods of extreme precision is essential for their future experimental achievement. Therefore, the *ab initio* study using RHF (Restrict Hartree-Fock method) [4-13] and the set of basis used is CC-pVTZ [10-14] and 6-311G** (3df, 3pd) [7,14-37].

The calculation of the Raman spectrum of the nano-molecule Genesis has the purpose of deepening the knowledge and characterization of this. The work characterizes the Raman spectrum of

the nano-molecule $C_{13}H_{20}BeLi_2SeSi$. Calculations obtained in the *ab initio* RHF (Restrict Hartree-Fock method) [4-13]. The set of basis used that have are CC-pVTZ [10-14] and 6-311G** (3df, 3pd) [7, 14-18].

Materials and Methods

Hartree-fock methods

The Hartree-Fock self-consistent method [4-13] is based on the one-electron approximation in which the motion of each electron in the effective field of all the other electrons is governed by a one-particle Schrodinger equation. The Hartree-Fock approximation takes into account of the correlation arising due to the electrons of the same spin, however, the motion of the electrons of the opposite spin remains uncorrelated in this approximation. The methods beyond self-consistent field methods, which treat the phenomenon associated with the many-electron system properly, are known as the electron correlation methods. One of the approaches to electron correlation is the Møller-Plesset (MP) [4-18] perturbation theory in which the Hartree-Fock energy is improved by obtaining a perturbation expansion for the correlation energy. [4,5]

However, MP calculations are not variational and can produce an energy value below the true energy [4,5]. The exchange-correlation energy is expressed, at least formally, as a functional of the resulting electron density distribution, and the electronic states are solved for self-consistently as in the Hartree-Fock approximation [4-13].

The full Hartree-Fock equations are given by

$$\epsilon_i \Psi_i(r) = \left(-\frac{1}{2} \nabla^2 V_{ion}(r) \right) \Psi_i(r) + \sum_j \int dr' \frac{|\Psi_j(r')|^2}{|r-r'|} \Psi_i(r) - \sum_j \delta_{\sigma_i, \sigma_j} \int dr' \frac{\Psi_j^*(r') \Psi_i(r')}{|r-r'|} \Psi_j(r) \quad (1)$$

The minimal basis sets are not flexible enough for accurate representation of orbitals. Using multiple functions to represent each orbital, have the double-zeta basis set allows us to treat each orbital separately when we conduct the Hartree-Fock calculation:

$$\Phi_{2s}(r) = \Phi_{2s}^{STO}(r, \xi_1) + d \Phi_{2s}^{STO}(r, \xi_2) \quad (2)$$

In Equation (2) 2s atomic orbital expressed as the sum of two STOs (Slater type orbitals) [4,5]. The two equations are the same except for the value of ξ which accounts for how large the orbital is. The constant d determines how much each STO will count towards the final orbital [4,5].

The vast literature associated with these methods suggests that the following is a plausible hierarchy :

$$HF \ll MP2 < CISD < CCSD < CCSD(T) < FCI \quad (3)$$

The extremes of 'best', FCI, and 'worst', HF, are irrefutable, but the intermediate methods are less clear and depend on the type of chemical problem being addressed. The use of HF [4-13] in the case of FCI was due to the computational cost.

Hardware and Software

For calculations a computer models was used: Intel® Core™ i3-3220 CPU @ 3.3 GHz x 4 processors [38], Memory DDR3 4GB, HD SATA WDC WD7500 AZEK-00RKA0 750.1GB and DVD-RAM SATA GH24NS9 ATAPI, Graphics Intel® Ivy Bridge [1].

The *ab initio* calculations have been performed to study the equilibrium configuration of C₁₃H₂₀BeLi₂SeSi molecule using the GAMESS [14,15]. The set of programs Mercury 3.8 [39], Avogadro [40,41] are the advanced semantic chemical editor, visualization, and analysis platform and GAMESS [14,15] is a computational chemistry software program and stands for General Atomic and Molecular Electronic Structure System [14,15] set of programs.

For calculations of computational dynamics, the Ubuntu Linux version 16.10 system was used [42]. The Graphic was edited in Origin software [43], for comparison of the spectra obtained in the set of bases used.

Results

Our results takes place from the findings of the molecular dynamics of bio-inorganic nano-molecule C₁₃H₂₀BeLi₂SeSi. The results were summarized and shown in Figures 1 & 2, Tables 1 & 2.

Nano-molecule Kurumi

The Figure 1 representation of the molecular structure of C₁₃H₂₀BeLi₂SeSi/C₁₃H₁₉BeLi₂SeSi, Nano-molecule Kurumi, 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2 lithacyclopropane.

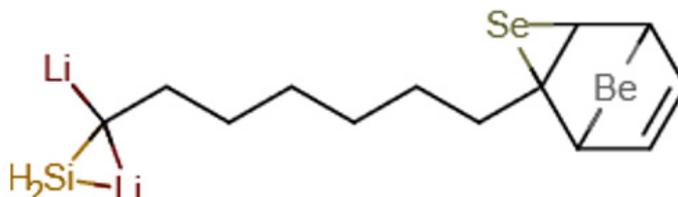


Figure 1: Representation of the molecular structure of C₁₃H₁₉BeLi₂SeSi, Nano-molecule Kurumi, 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane, obtained through computer via *ab initio* calculation method RHF/CC-pVTZ.

Raman spectrum

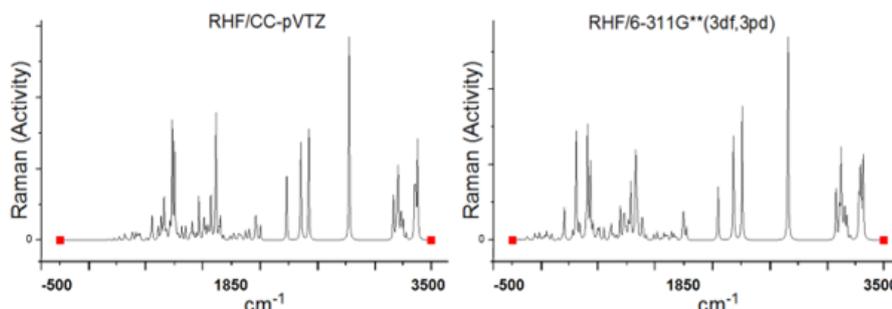


Figure 2: Representation of the Raman spectrum of C₁₃H₂₀BeLi₂SeSi - Frequency (cm-1) for Raman scattering activities (SR, Å⁴/amu) -using computer programs GAMESS, in the *ab initio* for the RHF method, in sets of basis RHF/CC-pVTZ in left and 6-311G**(3df, 3pd) in right.

In Figure (2) we have representation of the Raman spectrum of C₁₃H₂₀BeLi₂SeSi - Nano-molecule Kurumi, 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane.

Frequency (cm-1) for Raman scattering activities (SR, Å⁴/amu) -using computer programs GAMESS, in the *ab initio* for the RHF method, in sets of basis RHF/CC-pVTZ in left and 6-311G**(3df, 3pd) in right, obtained using computer software GAMESS. The Graphic

edited in Origin software, for comparison of the spectra obtained in the set of bases used.

RHF/CC-pVTZ

The Table 1 contains the frequencies (cm^{-1}) for Raman scattering activities (SR, $\text{\AA}^4/\text{amu}$) of the Nano-molecule Kurumi, 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane via *ab initio* methods, set base RHF/CC-pVTZ for the infrared spectrum.

The highest for Raman scattering activities peaks are in the frequency 708 cm^{-1} with 8.448529382 $\text{\AA}^4/\text{amu}$, 732 cm^{-1} with 6.968083358 $\text{\AA}^4/\text{amu}$, 1,180 cm^{-1} with 8.947657695 $\text{\AA}^4/\text{amu}$, 2,180 cm^{-1} with 7.796950601 $\text{\AA}^4/\text{amu}$ and 3,348 cm^{-1} with 7.107609729 $\text{\AA}^4/\text{amu}$ for RHF/CC-pVTZ.

RHF/6-311G**(3df,3pd)

The Table 2 contains the frequencies (cm^{-1}) for Raman scattering activities (SR, $\text{\AA}^4/\text{amu}$) of the Nano-molecule Kurumi, via *ab initio* methods, set base RHF/6-311G**(3df,3pd) for the infrared spectrum.

The highest for Raman scattering activities peaks are in the frequency 602 cm^{-1} with 7.279393384 $\text{\AA}^4/\text{amu}$, 707 cm^{-1} with 7.719121469 $\text{\AA}^4/\text{amu}$, 2,079 cm^{-1} with 6.915053417 $\text{\AA}^4/\text{amu}$, 2,163 cm^{-1} with 8.902805583 $\text{\AA}^4/\text{amu}$ and 3,094 cm^{-1} with 6.213759835 $\text{\AA}^4/\text{amu}$ for RHF/6-311G**(3df,3pd).

Discussion

The calculations made so far admit a seed molecule at this stage of the quantum calculations of the arrangement of the elements we have chosen, obtaining a highly reactive molecule with the shape polar-apolar-polar. Its structure has polarity at its ends, having the characteristic polar-apolar-polar. Even using a simple base set the polar-apolar-polar characteristic is predominant. The set of bases used that have the best compatible, more precise results are CC-pVTZ and 6-311G (3df, 3pd). In the CC-pVTZ base set, the charge density in relation to 6-311G (3df, 3pd) is 50% lower. The structure of the bio-inorganic seed molecule for a biomembrane genesis that challenge the current concepts of a protective mantle structure of a

cell such as biomembrane to date is promising, challenging. Leaving to the biochemists their experimental synthesis.

The study evolves to construct a biomembrane from the seed molecule. The calculations default already performed admit a hydrophobic and hydrophilic molecule, the basis of the formation of a micelle and or biomembrane, as the default template. But kurumi molecule is polar-apolar-polar characteristic is predominant, i.e. A hydrophilic-hydrophobic-hydrophilic molecule, thus presenting another standard for the construction of a biomembrane, which is even more innovative because a bio-inorganic molecule. Going beyond imagination, the most innovative and challenging proposal of the work advances the construction of a structure compatible with the formation of a «new DNA», based now on the seed molecule. Our discussion takes place from the findings of the molecular dynamics of bio-inorganic nano-molecule $\text{C}_{13}\text{H}_{20}\text{BeLi}_2\text{SeSi}$. The results were summarized and shown in Figures 1 & 2, Tables 1 & 2.

The Figure 1 representation of the molecular structure of $\text{C}_{13}\text{H}_{19}\text{BeLi}_2\text{SeSi}$, Nano-molecule Kurumi, 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane, obtained through computer via *ab initio* calculation method RHF/CC-pVTZ.

The Figure 2 represents of the Raman spectrum of $\text{C}_{13}\text{H}_{20}\text{BeLi}_2\text{SeSi}$ - Frequency (cm^{-1}) for Raman scattering activities (SR, $\text{\AA}^4/\text{amu}$) - using computer programs GAMESS, in the *ab initio* for the Restrict Hartree-Fock method, in sets of basis CC-pVTZ and 6-311G**(3df, 3pd), obtained using computer software GAMESS. Graphic edited in Origin software, for comparison of the spectra obtained in the set of bases used.

The Tables 1 & 2 present the Raman spectrum frequencies for CC-pVTZ and 6-311G**(3df, 3pd), respectively, for Raman scattering activities (SR, $\text{\AA}^4/\text{amu}$), $\text{SR} > 1$.

The highest for Raman scattering activities peaks are in the frequency 3,348 cm^{-1} with 7.107609729 $\text{\AA}^4/\text{amu}$ and 2,163 cm^{-1} with 8.902805583 $\text{\AA}^4/\text{amu}$, for CC-pVTZ and 6-311G**(3df, 3pd), respectively.

Table 1: Table contains the frequencies (cm^{-1}) for Raman scattering activities (SR, $\text{\AA}^4/\text{amu}$) of the $\text{C}_{13}\text{H}_{20}\text{BeLi}_2\text{SeSi}$ molecule via *ab initio* methods, set base RHF/CC-pVTZ for the infrared spectrum.

$\nu(\text{cm}^{-1})$	SR($\text{\AA}^4/\text{amu}$)						
492	1.776731	812	1.028877	1212	1.041326	3124	1.903406
556	1.002196	852	1.041603	1228	1.750528	3132	3.589672
588	1.72755	924	1.360705	1604	1.699802	3140	5.264159
596	1.146249	996	3.12066	1612	1.730788	3148	1.707891
612	1.638659	1004	1.241567	1660	1.055684	3164	1.250803
620	3.087802	1044	1.055248	2172	2.528493	3172	2.086607
628	1.303999	1052	1.632863	2180	7.796951	3180	1.003229
684	1.370946	1068	1.058814	2188	1.353183	3196	1.523681
700	1.941684	1092	1.09638	2604	2.449866	3316	3.894353
708	8.448529	1124	3.183402	2612	4.231962	3324	3.953024
716	2.009311	1132	1.198932	2620	4.275745	3332	3.687871

724	1.737035	1164	1.702475	2628	1.112317	3340	2.315845
732	6.968083	1172	3.720249	3084	1.454578	3348	7.10761
740	1.80891	1180	8.947658	3092	3.202109	3356	2.854032
748	1.090269	1188	1.75441	3116	1.435717	-	-

Table 2: Table contains the frequencies (cm⁻¹) for Raman scattering activities (SR, Å⁴/amu) of the C₁₃H₂₀BeLi₂SeSi molecule via *ab initio* methods, set base RHF/6-311G**(3df,3pd) for the infrared spectrum.

ν(cm ⁻¹)	SR(Å ⁴ /amu)						
490	2.182596	1050	1.851075	1932	1.885078	3094	6.21376
595	3.420969	1057	1.707548	1939	3.535241	3101	3.519756
602	7.279393	1092	1.388367	2072	1.463697	3108	1.427854
609	1.764814	1099	1.118466	2079	6.915053	3115	1.154649
630	1.192582	1106	1.109801	2086	4.240445	3122	1.346301
637	1.038282	1113	3.899045	2093	1.062849	3129	2.315457
693	1.755585	1120	1.974696	2156	2.115886	3136	1.096041
700	2.135401	1148	1.021344	2163	8.902806	3150	1.711815
707	7.719121	1155	3.520772	2170	2.324113	3262	3.23569
714	2.723003	1162	6.018009	2583	1.551622	3269	3.008913
721	1.36844	1169	3.541951	2590	5.920065	3276	5.031301
728	2.834444	1176	2.474677	2597	3.47486	3283	3.414571
735	5.297166	1183	1.335813	2604	2.774907	3290	2.106915
742	1.255979	1218	1.504666	3045	3.454342	3297	4.656712
756	1.287419	1225	1.55933	3052	1.894141	3304	5.694054
931	1.12492	1603	1.285718	3073	1.020319	3311	1.308788
1015	2.295633	1610	1.928284	3080	2.52559	-	-
1043	1.507847	1617	1.257005	3087	2.277247	-	-

It presents “fingerprint” between the intermediate frequency intervals presented in Tables 1 & 2.

Calculations obtained in the *ab initio* RHF method, on the set of basis used, indicate that the simulated molecule, C₁₃H₂₀BeLi₂SeSi, is acceptable by quantum chemistry. Its structure has polarity at its ends, having the characteristic polar-apolar-polar.

The 6-311G** (3df, 3pd) set of basis exhibits the characteristic of the central chain, with a Small density of negative charges, Near the ends of the Carbons of this. In the CC-pVTZ base set, the charge density in relation to 6-311G (3df, 3pd) is 50% lower. It is characterized infrared spectrum of the molecule C₁₃H₂₀BeLi₂SeSi, for absorbance and transmittance, in Hartree-Fock method in the set of bases CC-pVTZ and 6-311G (3df, 3pd). The dipole moments CC-pTZV are 3.69% bigger than 6-311G** (3df, 3pd).

The new nano-molecule Kurumi is well characterize computationally. As its scientific name 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane. Getting Kurumi name, which means boy in Tupi-Guarani language, which are indigenous inhabitants of southern Brazil.

Limitations

Our study has so far been limited to computational simulation via quantum chemistry, an applied theory. Our results and calculations are compatible and with the theory of quantum chemistry,

but their physical experimental verification depends on advanced techniques for their synthesis, obtaining laboratory for experimental biochemical.

Conclusion

The highest for Raman scattering activities peaks are in the frequency 3,348 cm⁻¹ with 7.107609729 Å⁴/amu and 2,163 cm⁻¹ with 8.902805583 Å⁴/amu, for CC-pVTZ and 6-311G** (3df, 3pd), respectively. The Raman spectrum was calculated, indicating the characteristic of the bioinorganic nano-molecule genesis. Now the challenge is to build the basic structure of the bio-inorganic membrane. From the unimaginable, going where our mind can take us and build a new DNA, that nanomolecule. Characterized its infrared spectrum and Raman. Quantically calculated, accepted by quantum chemistry parameters, with *ab initio* methods, in the bases CC-pVTZ and 6-311G ** (3df, 3pd). An experimental challenge to chemists. The new bio-inorganic nano-molecule C₁₃H₂₀BeLi₂SeSi/C₁₃H₁₉BeLi₂SeSi, is well characterize computationally. As its scientific name 3-lithio-3-(6-{3-selena-8-beryllatricyclo[3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane, getting Kurumi name, which means boy in Tupi-Guarani language, which are indigenous inhabitants of southern Brazil. As the bio-inorganic nano-molecule Kurumi is the basis for a new creation of a biomembrane, later calculations that challenge the current concepts of biomembrane should advance to such a purpose.

Acknowledgement

None.

Conflict of Interest

No conflict of interest.

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