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# RAMAN SPECTROSCOPY STUDY OF THE NANO MOLECULE $C_{13}H_{20}BeLi_2SeSi$ USING *AB INITIO* AND HARTREE-FOCK METHODS IN THE BASIS SET CC-PVTZ AND 6-311G\*\* (3DF, 3PD)

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**Abstract:** The work characterizes the Raman spectroscopy of the nano molecule  $C_{13}H_{20}BeLi_2SeSi$ . Calculations obtained in the *ab initio* restrict Hartree-Fock method, on the basis set was used to indicate that the simulated molecule  $C_{13}H_{20}BeLi_2SeSi$  features the structure polar-apolar-polar predominant. The basis set which was used that includes CC-pVTZ and 6-311G\*\* (3df, 3pd). In the CC-pVTZ basis 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 15.799 (Å). The Raman spectrum was calculated for indicating the characteristic of the nano molecule and their frequency ( $cm^{-1}$ ) were obtained in the basis set was used. The highest for Raman scattering activities peaks are in the frequency 3.348 ( $cm^{-1}$ ) with 7.107609729 ( $Å^4/amu$ ) and 2.163 ( $cm^{-1}$ ) with 8.902805583 ( $Å^4/amu$ ) for CC-pVTZ and 6-311G\*\* (3df, 3pd), respectively. As the bio-inorganic molecule  $C_{13}H_{20}BeLi_2SeSi$  is the basis set for a new creation of a biomembrane, later calculations that challenge the current concepts of biomembrane should advance to such a purpose.

**Keywords:** Biomembrane,  $C_{13}H_{20}BeLi_2SeSi$ , CC-pVTZ, Hartree-Fock Method, Nano Molecule, Raman Spectroscopy, 6-311G\*\* (3df, 3pd).

## 1. Introduction

Studies did not reveal any works with characteristics studied here. There is an absence of a referential of the theme, finding only one work in (Gobato et al., 2018) [1].

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) [2-14]. The basis set was used that includes CC-pVTZ [10-14] and 6-311G\*\* (3df, 3pd) [7, 15-25].

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 to date is promising and challenging. Leaving to the Biochemists their experimental synthesis. Structures of a liquid crystal such as a new membrane may occur, micelles [1, 26-64].

## 2. Methods

### 2.1. Hartree-Fock Methods

The full Hartree-Fock equations are given by:

$$\begin{aligned} \epsilon_i \psi_i(\mathbf{r}) = & \left( -\frac{1}{2} \nabla^2 + V_{\text{ion}}(\mathbf{r}) \right) \psi_i(\mathbf{r}) + \sum_j \int d\mathbf{r}' \frac{|\psi_j(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} \psi_i(\mathbf{r}) \\ & - \sum_j \delta_{\sigma_i \sigma_j} \int d\mathbf{r}' \frac{\psi_j^*(\mathbf{r}') \psi_i(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \psi_j(\mathbf{r}). \end{aligned} \quad (1)$$

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

$$HF \ll MP2 < CISD < CCSD < CCSD(T) < FCI \quad (2)$$

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 [2-14] in the case of FCI was due to the computational cost.

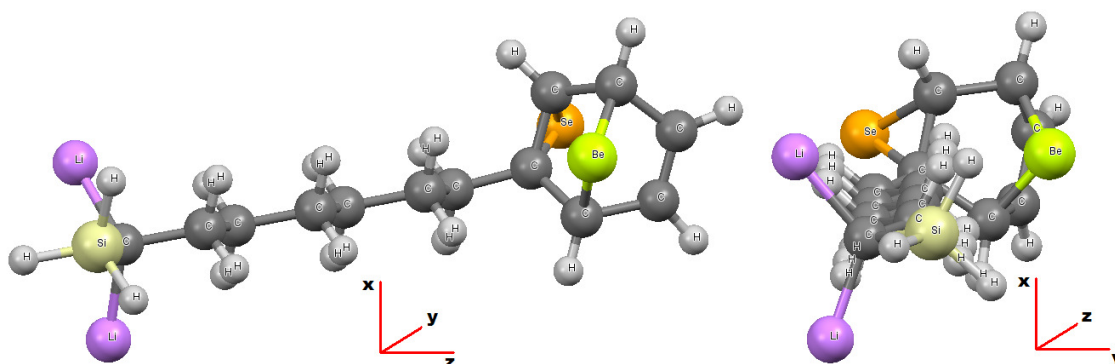
### 2.2. Hardware and Software

For calculations a computer models was used: Intel<sup>®</sup> Core<sup>™</sup> i3-3220 CPU @ 3.3 GHz x 4 processors [65], Memory DDR3 4 GB, HD SATA WDC WD7500 AZEK-00RKKA0 750.1 GB and DVD-RAM SATA GH24NS9 ATAPI, Graphics Intel<sup>®</sup> Ivy Bridge [66].

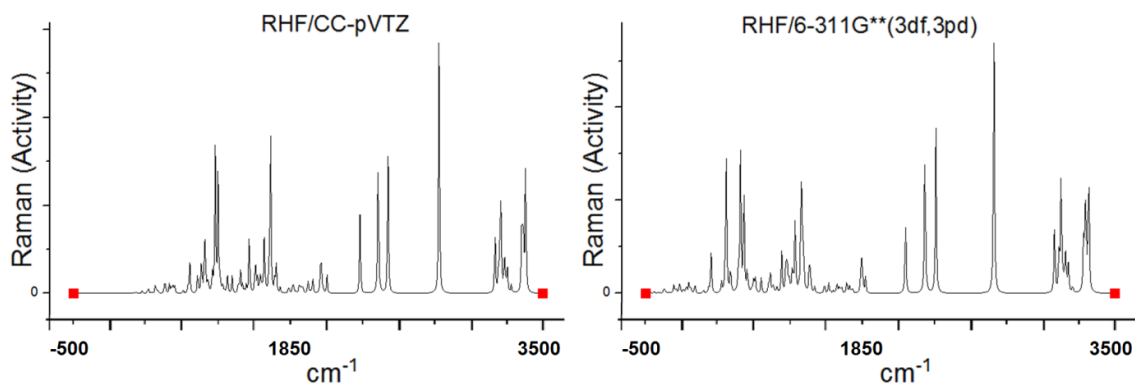
The *ab initio* calculations have been performed to study the equilibrium configuration of  $C_{13}H_{20}BeLi_2SeSi$  molecule using the GAMESS [15, 20]. The set of programs GaussView 5.0.8 [67], Mercury 3.8 [68], Avogadro [69, 70] are the advanced semantic chemical editor, visualization, and analysis platform and GAMESS [15, 20] is a computational chemistry software program and stands for General Atomic and Molecular Electronic Structure System [15, 20] set of programs.

For calculations of computational dynamics, the Ubuntu Linux version 16.10 system was used. [71] The Graphic was edited in origin software, for comparison of the spectra obtained in the basis set was used. [72-284]

### 3. Results



**Figure 1.** Representation of the molecular structure of  $C_{13}H_{20}BeLi_2SeSi$ , obtained through computer via *ab initio* calculation method RHF/CC-pVTZ. [2-14] sets basis obtained using computer programs GAMESS [15, 20]. Images obtained in the software Mercury 3.8 [68]. Represented in bluish gray color the atom of silicon, in the purple color lithium, in the lemon yellow color beryllium, in the orange the selenium, in dark gray color carbon and in light gray color hydrogen. The image from left to right has a  $90^\circ$  rotation in the YZ plane, anti-clockwise. [1]



**Figure 2.** Representation of the Raman spectrum of  $C_{13}H_{20}BeLi_2SeSi$  - Frequency ( $cm^{-1}$ ) for Raman scattering activities (SR,  $\text{\AA}^4/\text{amu}$ ) -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. Graphic edited in origin software, for comparison of the spectra obtained in the basis set was used.

**Table 1.** Table containing the frequency ( $\text{cm}^{-1}$ ) 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, basis set RHF/CC-pVTZ for the infrared spectrum.

$\nu(\text{cm}^{-1})$	SR( $\text{\AA}^4/\text{amu}$ )	$\nu(\text{cm}^{-1})$	SR( $\text{\AA}^4/\text{amu}$ )	$\nu(\text{cm}^{-1})$	SR( $\text{\AA}^4/\text{amu}$ )	$\nu(\text{cm}^{-1})$	SR( $\text{\AA}^4/\text{amu}$ )
492	1.776730604	812	1.028877220	1212	1.041326344	3124	1.903405815
556	1.002195612	852	1.041603296	1228	1.750528008	3132	3.589671617
588	1.727549781	924	1.360704999	1604	1.699802334	3140	5.264159067
596	1.146248919	996	3.120659749	1612	1.730787547	3148	1.707890875
612	1.638659371	1004	1.241567405	1660	1.055684108	3164	1.250803021
620	3.087802356	1044	1.055247752	2172	2.528493226	3172	2.086606981
628	1.303998749	1052	1.632862637	2180	7.796950601	3180	1.003229327
684	1.370945770	1068	1.058814167	2188	1.353182724	3196	1.523680735
700	1.941683802	1092	1.096380258	2604	2.449865964	3316	3.894352743
708	8.448529382	1124	3.183402401	2612	4.231962257	3324	3.953024127
716	2.009310809	1132	1.198931550	2620	4.275744845	3332	3.687870867
724	1.737034728	1164	1.702474909	2628	1.112316620	3340	2.315844592
732	6.968083358	1172	3.720249465	3084	1.454577799	3348	7.107609729
740	1.808910110	1180	8.947657695	3092	3.202109137	3356	2.854032181
748	1.090269379	1188	1.754410154	3116	1.435717251	-	-

**Table 2.** Table containing the frequency ( $\text{cm}^{-1}$ ) for Raman scattering activities ( $\text{SR}, \text{\AA}^4/\text{amu}$ ) of the  $\text{C}_{13}\text{H}_{20}\text{BeLi}_2\text{SeSi}$  molecule via *ab initio* methods, basis set RHF/6-311G\*\*(3df,3pd) for the infrared spectrum.

$\nu(\text{cm}^{-1})$	$\text{SR}(\text{\AA}^4/\text{amu})$	$\nu(\text{cm}^{-1})$	$\text{SR}(\text{\AA}^4/\text{amu})$	$\nu(\text{cm}^{-1})$	$\text{SR}(\text{\AA}^4/\text{amu})$	$\nu(\text{cm}^{-1})$	$\text{SR}(\text{\AA}^4/\text{amu})$
490	2.182595992	1050	1.851075321	1932	1.885077651	3094	6.213759835
595	3.420968896	1057	1.707548488	1939	3.535241007	3101	3.519756467
602	7.279393384	1092	1.388367323	2072	1.463696578	3108	1.427853794
609	1.764814173	1099	1.118465541	2079	6.915053417	3115	1.154649320
630	1.192581642	1106	1.109800606	2086	4.240445361	3122	1.346300787
637	1.038282391	1113	3.899044667	2093	1.062849049	3129	2.315456625
693	1.755584759	1120	1.974696491	2156	2.115886063	3136	1.096040616
700	2.135401292	1148	1.021343875	2163	8.902805583	3150	1.711814612
707	7.719121469	1155	3.520772454	2170	2.324112769	3262	3.235690369
714	2.723002570	1162	6.018008677	2583	1.551622068	3269	3.008913115
721	1.368440323	1169	3.541951140	2590	5.920064859	3276	5.031300992
728	2.834443522	1176	2.474677204	2597	3.474860306	3283	3.414570790
735	5.297166302	1183	1.335813469	2604	2.774906909	3290	2.106914946
742	1.255979452	1218	1.504666259	3045	3.454342110	3297	4.656712492
756	1.287419280	1225	1.559329727	3052	1.894141214	3304	5.694053509
931	1.124920117	1603	1.285718149	3073	1.020319159	3311	1.308788386
1015	2.295632761	1610	1.928283613	3080	2.525590242	-	-
1043	1.507847235	1617	1.257004796	3087	2.277247129	-	-

#### 4. Discussions

The Figure (2) represents of the Raman spectrum of  $\text{C}_{13}\text{H}_{20}\text{BeLi}_2\text{SeSi}$  - Frequency ( $\text{cm}^{-1}$ ) for Raman scattering activities ( $\text{SR}, \text{\AA}^4/\text{amu}$ ) - 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 basis set was used.

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

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

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

Calculations obtained in the *ab initio* RHF method, on the basis set was used, indicate that the simulated molecule,  $\text{C}_{13}\text{H}_{20}\text{BeLi}_2\text{SeSi}$ , is acceptable by quantum chemistry. Its structure has polarity at its ends, having the characteristic polar-apolar-polar.

The 6-311G\*\*(3df, 3pd) basis set 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  $C_{13}H_{20}BeLi_2SeSi$ , for absorbance and transmittance, in Hartree-Fock method in the basis set CC-pVTZ and 6-311G (3df, 3pd). The dipole moments CC-pTZV are 3.69% bigger than 6-311G\*\* (3df, 3pd).

## 5. Conclusions

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

The Raman spectrum was calculated, indicating the characteristic of the 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.

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