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Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR) Spectroscopy Study of the Nano Molecule $C_{13}H_{20}BeLi_2SeSi$ Using *ab initio* and Hartree-Fock Methods in the Basis Set RHF/CC-pVTZ and RHF/6-311G** (3df, 3pd): An Experimental Challenge to Chemists

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ABSTRACT: The work characterizes the ATR-FTIR 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 RHF/CC-pVTZ and RHF/6-311G** (3df, 3pd). In the RHF/CC-pVTZ basis set, the charge density in relation to RHF/6-311G** (3df, 3pd) is 50% lower. The length of the molecule $C_{13}H_{20}BeLi_2SeSi$ is of 15.799 (Å). The ATR-FTIR 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 ATR-FTIR 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 RHF/CC-pVTZ and RHF/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, $C_{13}H_{20}BeLi_2SeSi$, RHF/CC-pVTZ, Hartree-Fock Method, Nano Molecule, ATR-FTIR Spectroscopy, RHF/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 ATR-FTIR spectrum of the nano-molecule Genesis has the purpose of deepening the knowledge and characterization of this. The work characterizes the ATR-FTIR 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 RHF/CC-pVTZ [10-14] and RHF/6-311G** (3df, 3pd) (Figure (1)) [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:

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

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

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

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® Core™ 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® 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. [72-295].

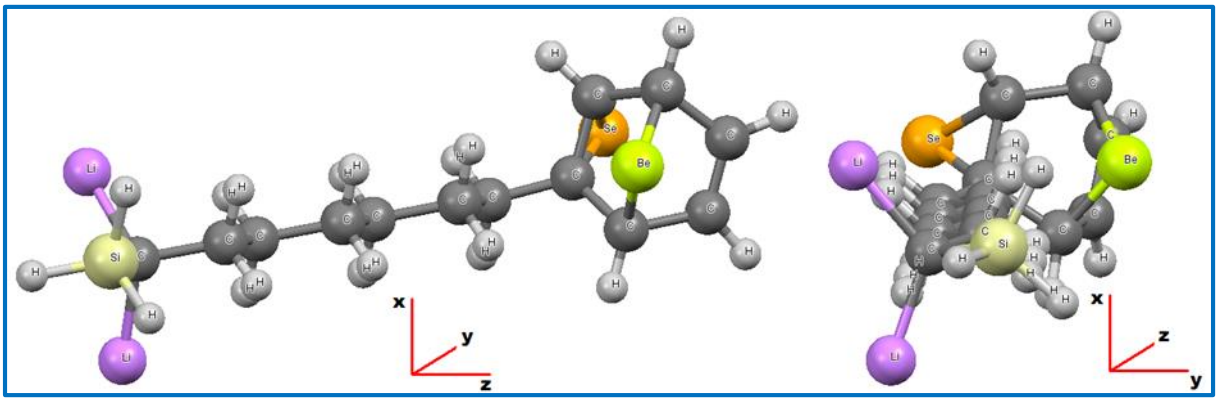
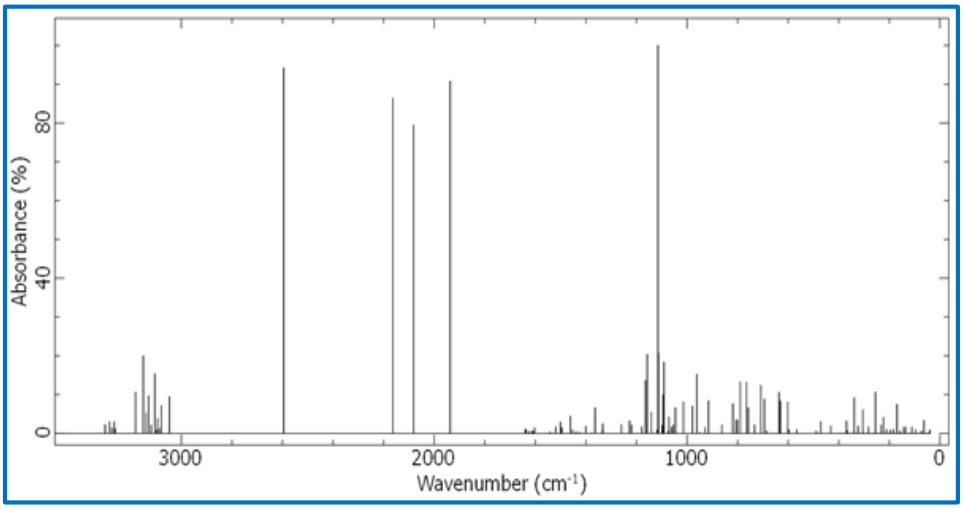


Figure 1. Representation of the molecular structure of $C_{13}H_{20}BeLi_2SeSi$, obtained through computer via ab initio calculation method RHF/CC-pVTZ. [2-14] sets basis obtained using computer programs GAMESS [15, 20]. Images obtained in the software Mercury 3.8 [68]. Represented in bluish gray color 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 90º rotation in the YZ plane, anti-clockwise. [1]



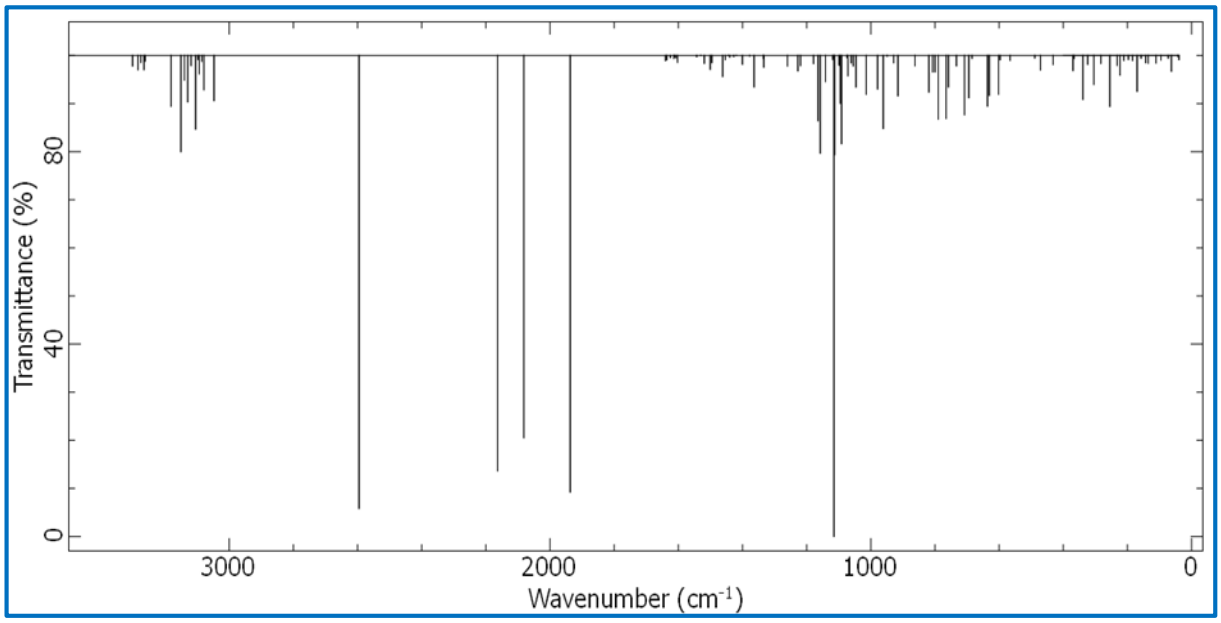


Figure 2. Characteristic ATR-FTIR spectrum is obtained using the *ab initio* HF method for the in basis set RHF/6-311G**(3df,3pd) is obtained using computer software GAMESS [7]. Image is created by Avogadro software.

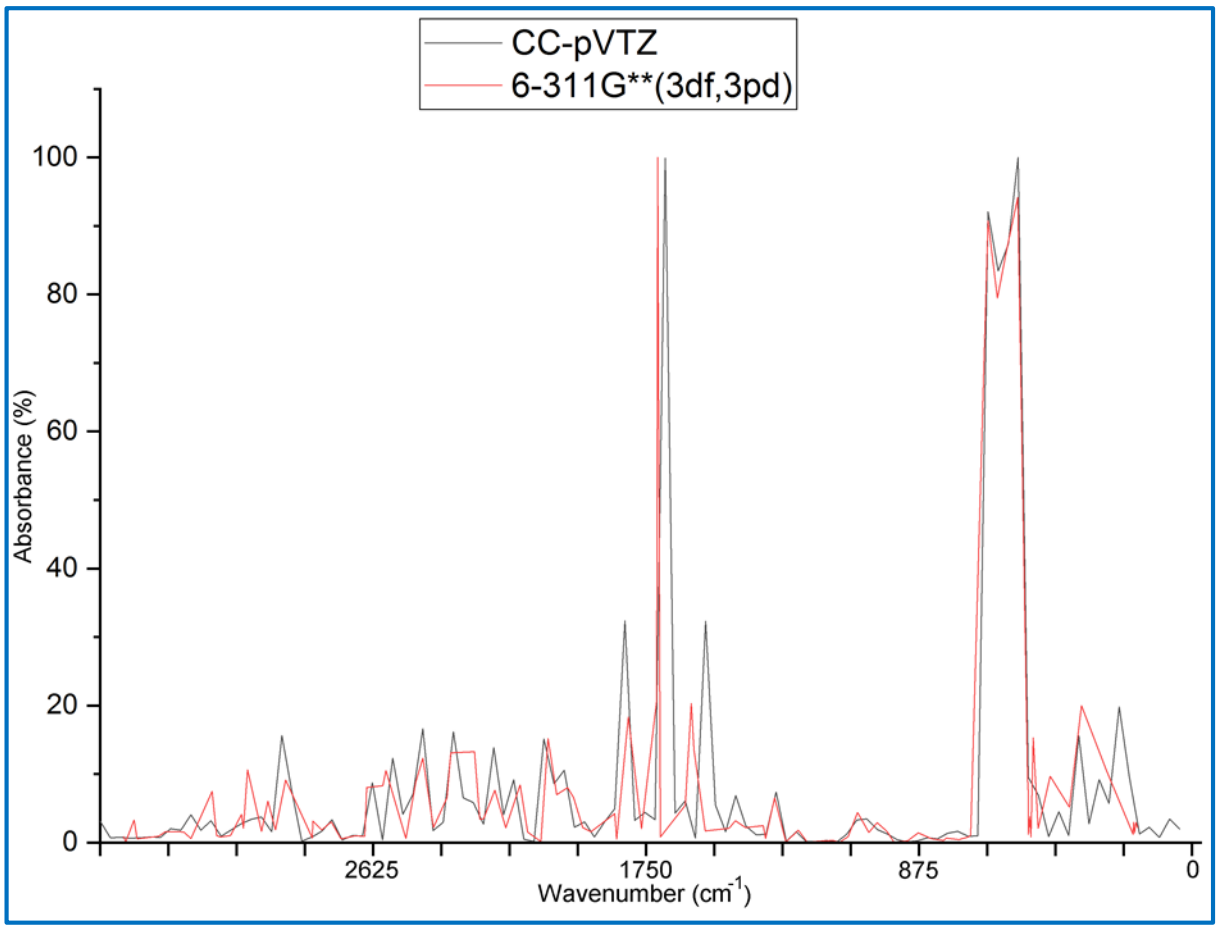


Figure 3. ATR-FTIR spectrum is obtained using the *ab initio* for the RHF method, in basis set RHF/6-311G**(3df,3pd) in black color and 6-311G**(3df, 3pd) in red color is obtained using computer software GAMESS.

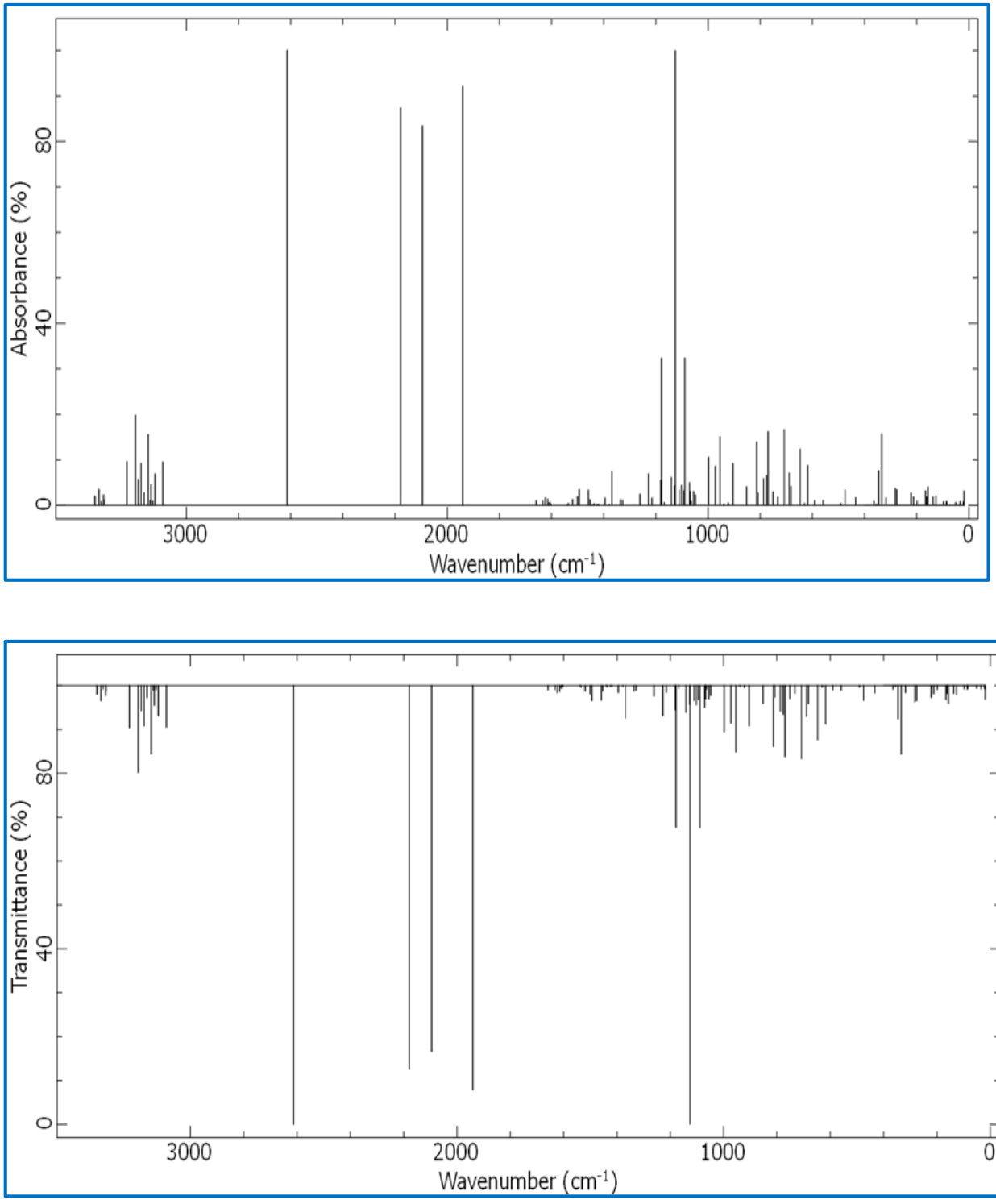


Figure 4. Characteristic ATR-FTIR spectrum is obtained using the *ab initio* HF method for the RHF [5-6, 27-32] in basis set CC-pVTZ [66-70] is obtained using computer software GAMESS [7]. Image is created by Avogadro software.

Table 1. **Table containing the frequency (cm^{-1}) for intensity (km/mol*)* of the $C_{13}H_{20}BeLi_2SeSi$ molecule via *ab initio* methods, basis set RHF/CC-pVTZ [66, 67, 68, 69, *70] for the ATR-FTIR spectrum.***

υ(cm-1)	I(km/mol)	υ(cm-1)	I(km/mol)	υ(cm-1)	I(km/mol)	υ(cm-1)	I(km/mol)	υ(cm-1)	I(km/mol)
18.3102	3.12029	433.7770	1.66974	953.8260	15.12960	1335.6300	1.20528	1940.7000	92.08140
21.8078	0.71641	474.6210	3.33766	972.1280	8.56993	1368.6100	7.38902	2094.8200	83.41340
33.8524	0.77400	490.5660	0.39700	998.0240	10.53800	1377.9600	0.19303	2178.4300	87.37120
50.7492	0.63010	558.7220	1.05878	1048.5900	2.26512	1394.9300	1.58394	2613.3900	100.00000
84.5077	0.72158	590.9540	1.00084	1055.4600	3.03114	1418.8000	0.14913	3089.6700	9.49051
86.6290	0.81646	617.3720	8.74975	1064.3500	0.81462	1424.6000	0.17433	3120.0100	6.88461
97.8753	0.74488	630.2770	0.38728	1067.4200	3.02414	1436.4400	0.31307	3128.3300	0.89217
126.2300	2.04010	647.2610	12.35180	1071.0300	4.96342	1441.4700	0.07686	3135.2400	4.50814
137.2420	1.79910	682.220	4.12012	1089.2000	32.38290	1452.5600	1.20736	3138.7500	1.03164
157.2190	4.05892	689.180	7.07040	1094.5300	3.21532	1458.8700	3.30915	3146.5000	15.56620
162.2760	1.79850	707.7970	16.62920	1101.9000	4.36570	1493.8200	3.44459	3162.1200	2.74526
166.1550	3.18327	732.6220	1.76020	1110.7000	3.36370	1500.5100	1.90950	3173.1800	9.21057
198.8160	0.89883	750.9170	2.93531	1125.4400	99.91360	1519.2200	1.26635	3184.0800	5.71116
212.1870	1.86318	769.8590	16.18050	1127.2300	4.28880	1535.0400	0.44678	3194.9900	19.79120
221.4760	2.72144	776.5010	6.54948	1141.0000	6.09320	1539.7800	0.07426	3227.8700	9.59669
275.6740	3.41994	787.0040	5.83286	1168.1800	0.62429	1602.1900	0.25765	3316.2100	1.26114
282.5210	3.70827	807.7180	2.65830	1178.4600	32.30970	1605.8200	0.68637	3317.1900	2.26056
317.5550	1.59558	813.4530	13.89200	1181.3800	5.50813	1609.5000	0.52610	3327.0400	0.77109
334.0370	15.62020	852.3830	4.08084	1215.0900	1.56665	1614.8500	1.36610	3334.5400	3.46058
345.6910	7.59721	904.1890	9.17924	1227.7900	6.88714	1623.7700	1.61794	3350.0700	1.98841
355.2290	0.19418	922.2350	0.47511	1261.0900	2.41179	1632.4000	0.92053	-	-
364.0620	0.83481	939.4860	0.16712	1327.9000	1.12109	1658.7900	0.99144	-	-

Table 2. **Table containing the frequency (cm^{-1}) for intensity (km/mol) of the $C_{13}H_{20}BeLi_2SeSi$ molecule via ab initio methods, basis set RHF/6-311G**(3df,3pd) for the ATR-FTIR spectrum.**

υ(cm^{-1})	**I(km/mol)**	**υ(cm^{-1})**	**I(km/mol)**	**υ(cm^{-1})**	**I(km/mol)**	**υ(cm^{-1})**	**I(km/mol)**	**υ(cm^{-1})**	**I(km/mol)**
39.3690	0.88442	431.6630	1.86731	961.2390	15.18990	1335.2000	0.61688	1936.8100	90.76620
42.9230	0.17054	471.0440	3.03500	978.6680	6.97516	1363.7400	6.53782	2081.4900	79.45730
62.8276	3.28814	488.8260	0.53052	1014.2000	8.05159	1377.7200	0.11690	2163.2300	86.38250
72.7607	0.56446	565.7610	1.00387	1046.0600	6.55719	1400.1200	1.82204	2595.2400	94.17240

95.4188	0.93953	596.7290	0.90320	1054.4100	2.19171	1419.3300	0.02732	3047.1700	9.41218
110.8990	1.57280	601.6700	8.03745	1061.3600	1.55943	1427.2800	0.22738	3078.8700	7.12474
134.9660	1.59724	630.4860	8.28940	1071.3000	4.21379	1439.5600	0.32592	3085.2000	1.20834
143.0760	1.53324	636.1600	10.5322	1074.6700	0.45713	1444.6600	0.01565	3093.5400	3.80278
157.2930	0.56626	684.4380	0.59237	1091.0800	18.34260	1453.3800	0.89434	3097.2200	0.83218
169.6890	7.45772	694.3870	8.79184	1094.8200	9.94311	1461.7000	4.37660	3104.6000	15.30960
183.9920	1.02760	707.9310	12.31890	1099.3200	2.01902	1495.1500	1.47712	3118.7700	2.09616
196.8790	0.82397	732.9940	2.16414	1112.9700	20.63790	1500.4800	2.89203	3129.3600	9.65626
211.2970	1.02116	758.0280	6.54359	1114.8300	100.00000	1519.0400	1.63496	3139.2800	5.15606
223.0370	4.09832	765.1440	13.09780	1118.4500	0.82424	1530.0000	0.02538	3150.5300	19.99360
232.0380	2.05430	789.5390	13.26570	1141.2300	5.42491	1542.7200	0.26491	3181.2300	10.55820
254.8190	10.59520	800.1070	3.41912	1157.3900	20.3207	1602.4700	1.41178	3261.8500	1.17952
282.7950	1.64299	807.5460	3.44432	1164.5800	13.5674	1607.4500	0.51568	3265.5700	2.95239
304.7080	6.03544	818.8740	7.61634	1178.3700	1.67813	1612.6000	0.31253	3275.0900	1.44561
323.7190	1.83394	862.2680	2.15917	1219.2200	2.10679	1614.2400	0.64217	3284.3500	2.97161
338.6760	9.13437	915.2640	8.40579	1227.2900	3.20311	1624.6400	0.43792	3301.0100	2.20326
366.6460	0.63580	928.7170	1.53060	1259.7100	2.20450	1635.2700	0.87439	-	-
369.5700	3.13170	949.1460	0.13393	1333.4400	2.44035	1639.7600	1.06541	-	-

4. Discussions

The Figures (2-4) represent of the ATR-FTIR spectrum of $C_{13}H_{20}BeLi_2SeSi$ - Frequency (cm^{-1}) for ATR-FTIR scattering activities (SR, $Å^4$/amu) - using computer programs GAMESS, in the *ab initio* for the Restrict Hartree-Fock method, in sets of basis RHF/CC-pVTZ and RHF/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 ATR-FTIR spectrum frequencies for RHF/CC-pVTZ and RHF/6-311G** (3df, 3pd), respectively, for ATR-FTIR scattering activities (SR, Å4/amu), *SR > 1*.

The highest for ATR-FTIR 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 RHF/CC-pVTZ and RHF/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, $C_{13}H_{20}BeLi_2SeSi$, is acceptable by quantum chemistry. Its structure has polarity at its ends, having the characteristic polar-apolar-polar.

The RHF/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 RHF/CC-pVTZ base set, the charge density in relation to 6-311G (3df, 3pd) is 50% lower. It is characterized ATR-FTIR spectrum of the molecule $C_{13}H_{20}BeLi_2SeSi$, for absorbance and transmittance, in Hartree-Fock method in the basis set RHF/CC-pVTZ and 6-311G (3df, 3pd). The dipole moments CC-pTZV are 3.69% bigger than RHF/6-311G** (3df, 3pd).

5. Conclusions

The highest for ATR-FTIR 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 RHF/CC-pVTZ and RHF/6-311G** (3df, 3pd), respectively.

The ATR-FTIR 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 nanomollecule. Characterized its ATR-FTIR spectrum and ATR-FTIR. Quantically calculated, accepted by quantum chemistry parameters, with *ab initio* methods, in the bases RHF/CC-pVTZ and 6-311G ** (3df, 3pd).

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