American Journal of Quantum Chemistry and Molecular Spectroscopy
2018; 2(1): 9-17
http://www.sciencepublishinggroup.com/j/ajqcms
doi: 10.11648/j.ajqcms.20180201.12

Spectroscopy and Dipole Moment of the Molecule $C_{13}H_{20}BeLi_2SeSi$ via Quantum Chemistry Using *Ab initio*, Hartree-Fock Method in the Base Set CC-pVTZ and 6-311G** (3df, 3pd)

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To cite this article:
Ricardo Gobato, Marcia Regina Risso Gobato, Alireza Heidari, Abhijit Mitra. Spectroscopy and Dipole Moment of the Molecule $C_{13}H_{20}BeLi_2SeSi$ Via Quantum Chemistry Using *Ab initio*, Hartree-Fock Method in the Base Set CC-pVTZ and 6-311G** (3df, 3pd). *American Journal of Quantum Chemistry and Molecular Spectroscopy*. Vol. 2, No. 1, 2018, pp. 9-17. doi: 10.11648/j.ajqcms.20180201.12

Received: July 24, 2018; **Accepted**: September 3, 2018; **Published**: October 4, 2018

Abstract: The work characterizes the electric dipole moment and the infrared spectrum of the molecule $C_{13}H_{20}BeLi_2SeSi$. Calculations obtained in the ab initio RHF (Restrict Hartree-Fock) method, on the set of basis used indicate that the simulated molecule $C_{13}H_{20}BeLi_2SeSi$ features the structure polar-apolar-polar predominant. The set of basis used that have 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 length of the molecule $C_{13}H_{20}BeLi_2SeSi$ is of 15.799Å. The magnitude of the electric dipole moment $|\vec{p}|$ total obtained was p = 4.9771 Debye and p = 4.7936 Debye, perpendicular to the main axis of the molecule, for sets basis CC-pVTZ and 6-311**(3df, 3pd), respectively. The infrared spectra for absorbance and transmittance and their wavenumber (cm^{-1}) were obtained in the set of bases used. The infrared spectrum for Standard CC-pVTZ shows peaks in transmittance with Intensity (I), at wavenumber 1,125.44 cm^{-1}, 1,940.70 cm^{-1}, 2,094.82 cm^{-1}, 2,178.43 cm^{-1}, 2,613.99 cm^{-1} and transmittance 433.399 km/mol, 399.425 km/mol, 361.825 km/mol, 378.993 km/mol, 433.774 km/mol, respectively. While the infrared spectrum for Standard 6-311G**(3df, 3pd), shows peaks in transmittance, at wavelengths 1,114.83 cm^{-1}, 1,936.81 cm^{-1}, 2,081.49 cm^{-1}, 2,163.23 cm^{-1}, 2,595.24 cm^{-1} and transmittance 434.556 km/mol, 394.430 km/mol, 345.287 km/mol, 375.381 km/mol, 409.232 km/mol, respectively. It presents "fingerprint" between the intervals (680 cm^{-1} and 1,500 cm^{-1}) and (3,250 cm^{-1} and 3,500 cm^{-1}). The dipole moments CC-pTZV are 3.69% bigger than 6-311G** (3df, 3pd). As the bio-inorganic molecule $C_{13}H_{20}BeLi_2SeSi$ is the basis for a new creation of a bio-membrane, later calculations that challenge the current concepts of biomembrane should advance to such a purpose.

Keywords: 6-311G** (3df, 3pd), Biomembrane, CC-pTZV, Dipole Moment, Infrared Spectra, Restrict Hartree-Fock

1. Introduction

The work characterizes the electric dipole moment and the infrared spectrum of the molecule $C_{13}H_{20}BeLi_2SeSi$. [1] Using a computational simulation using ab initio methods, RHF (Restrict Hartree-Fock), [2-9] set of basis CC-pVTZ [10-14] and 6-311G (3df, 3pd) [7, 15-21].

Preliminary bibliographic 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 R. Gobato et al., 2018 [1]. To construct such a molecule, which was called a seed molecule, quantum chemistry was used by ab initio methods [2, 3, 15]. The equipment used was of the

Biophysics laboratory built specifically for this task. The results were satisfactory.

The ab initio calculations, by RHF [2-9] in the CC-pVTZ [10-14] and 6-311G (3df, 3pd) [7, 15-21], sets basis was shown to be stable by changing its covalent cyclic chain linkages, which was expected, Figure (2). The set of basis used was that of Ahlrichs and coworkers the TZVP keywords refer to the initial formations of the split valence and triple zeta basis sets from this group [22, 23].

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, challenging. Leaving to the Biochemists their experimental synthesis. The quantum calculations must continue to obtain the structure of the bio-inorganic biomenbrane. The following calculations, which are the computational simulation via Mm+, QM/MM, should indicate what type of structure should form. Structures of a liquid crystal such as a new membrane may occur, micelles. [1, 24-62]

2. Methods

2.1. Hartree-Fock Methods

Hartree-Fock theory is one the simplest approximate theories for solving the many-body Hamiltonian. [2-9].

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 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. [63, 64] The use of HF in the case of FCI was due to the computational cost. [1, 24-62]

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]

3. Results

3.1. Figures, Graphics and Table

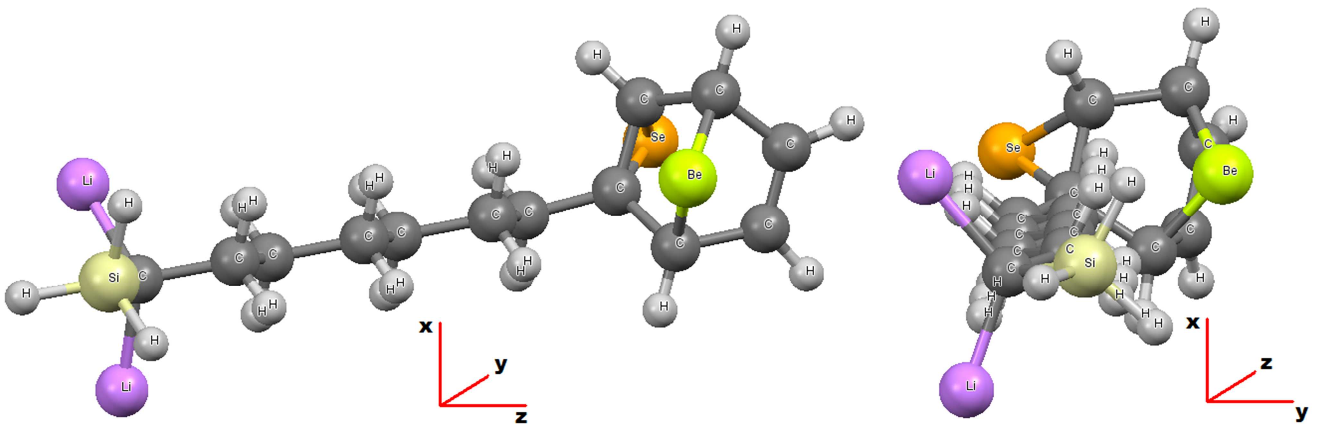

Figure 1. *Representation of the molecular structure of $C_{13}H_{20}BeLi_2SeSi$, obtained through computer via ab initio calculation method RHF [2-9], CC-pVTZ [10-14] sets basis obtained using computer programs GAMESS [15, 20]. Images obtained in the software Mercury 3.8 [68]. Represented in bluish 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 degree rotation in the YZ plane, anti-clockwise.*

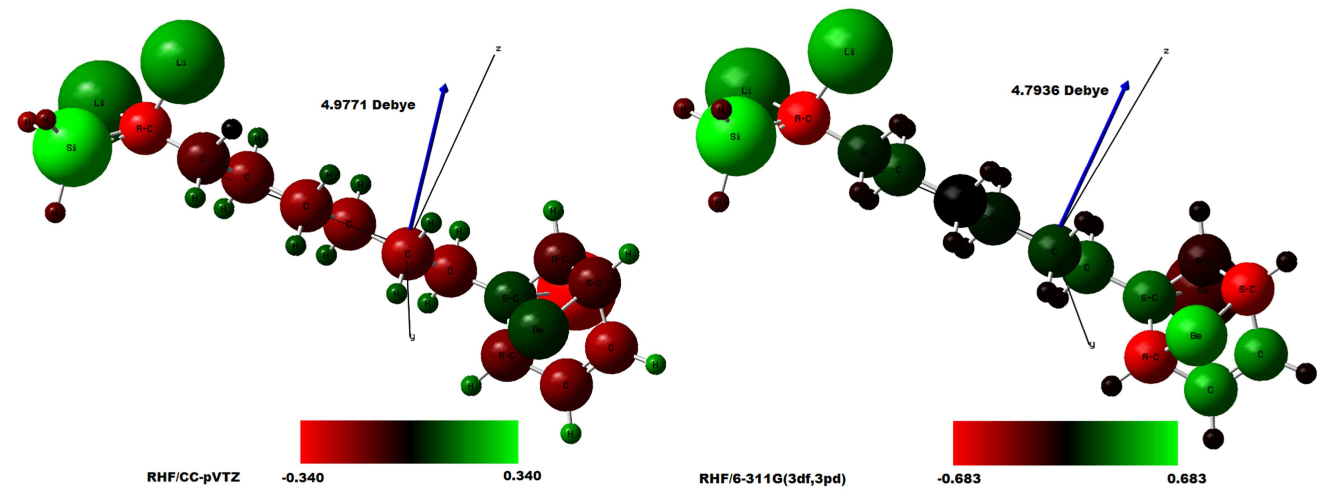

Figure 2. *Molecule bio-inorganic $C_{13}H_{20}BeLi_2SeSi$ after dynamics obtained through computer via ab initio calculation method RHF [2-9] in sets of basis obtained using computer software GAMESS [15, 20]. The length of the molecule $C_{13}H_{20}BeLi_2SeSi$ obtained in the base CC-pVTZ [10-14] is of 15.799Å. Represented in green color the positive charge, passing through the absence of color - black - zero charge, for the positive charge red color. A $\Delta\delta$ = 0.680 a.u. of CC-pVTZ [10-14] and $\Delta\delta$ = 1.366 a.u. of 6-311**(3df, 3pd) [7, 15-21], were the elemental charge e (e = ±1,607 x 10^{-19} C). Images obtained in the software Gaussview, Version 5, 2009 [67].*

Table 1. *Table containing the dipole moments of the $C_{13}H_{20}BeLi_2SeSi$ molecule via ab initio methods. [1, 24-62]*

Methods/Base	Dipole moment (Debye)			Total	Charge (a. u.)	
	X	Y	Z		δ±	Δδ
RHF/CC-pVTZ [10-14]	1.0338	1.6160	4.5925	4.9771	0.340	0.680
RHF/6-311G(3df, 3pd)[7, 15-21]	0.8366	1.0963	4.5910	4.7936	0.683	1.366

Selects Stuttgart potentials for Z > 2. MC-311G is a synonym for 6-311G. [7]. The elemental charge e (e = ±1,607 x 10^{-19} C) [1, 24-62].

*3.2. Spectroscopy for RHF/CC-pVTZ and RHF/6-311G** (3df, 3pd)*

3.2.1. RHF/CC-pVTZ

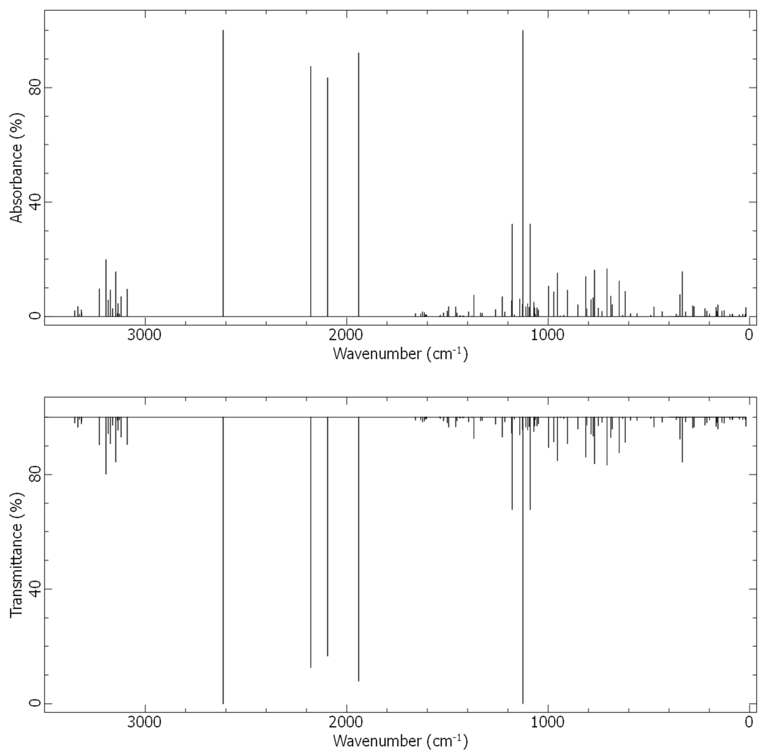

Figure 3. *Characteristic infrared spectrum in absorbance and transmittance obtained using the ab initio HF method for the RHF [5-6, 27, 28, 29, 30, 31, 32] in sets of basis CC-pVTZ [10-14] obtained using computer software GAMESS [15, 20]. Image created by Avogadro software [69, 70].*

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, set base RHF/CC-pVTZ [10-14] for the infrared 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	-	-

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

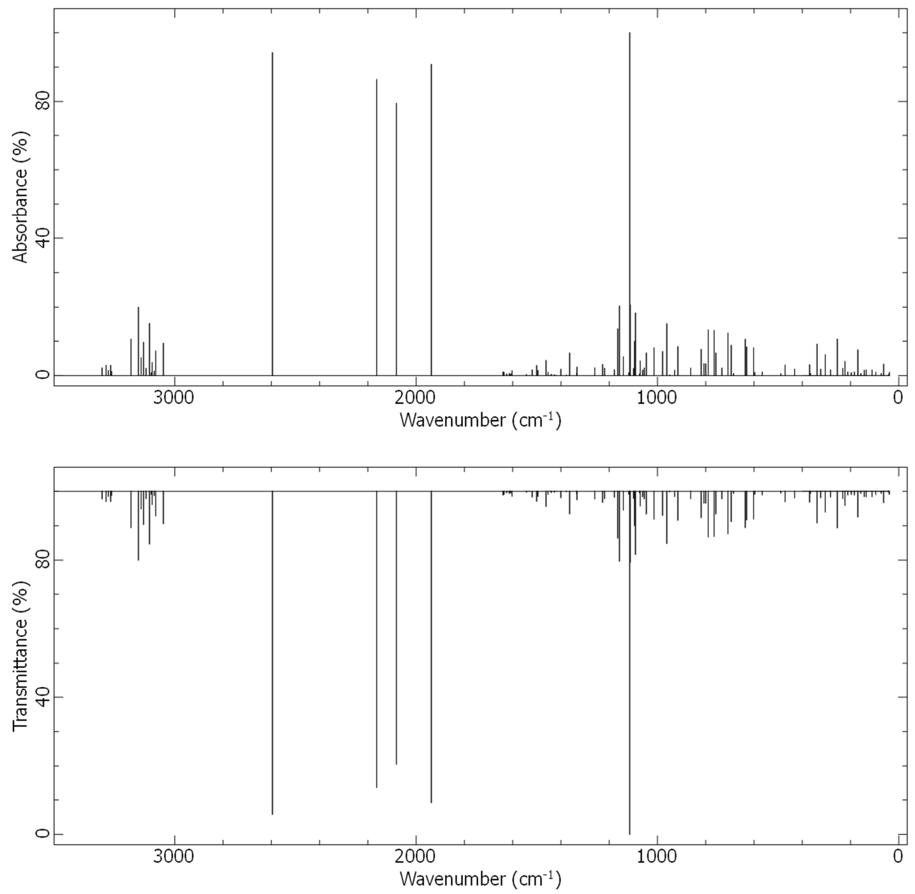

Figure 4. *Characteristic infrared spectrum in absorbance and transmittance obtained using the ab initio HF method for the RHF [2-9] in sets of basis RHF/6-311G**(3df, 3pd) [7, 15-21] obtained using computer software GAMESS [15, 20]. Image created by Avogadro software [69, 70].*

Table 3. *Table containing the frequency (cm^{-1}) for Intensity (km/mol) of the $C_{13}H_{20}BeLi_2SeSi$ molecule via ab initio methods, set base RHF/6-311G** (3df, 3pd) [7, 15-21] for the infrared 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 Figure (1) shows the final stable structure of the bio-inorganic $C_{13}H_{20}BeLi_2SeSi$ molecule obtained by an ab initio calculation with the method RHF (Restrict Hatrree-Fock), in sets of basis such as: 6-311G** (3df, 3pd) and CC-pVTZ.

As an example of analysis the set of basis CC-pVTV, with the charge distribution (Δδ) through it, whose charge variation is Δδ = 0.680 a.u. of elemental charge. In green color the intensity of positive charge displacement. In red color the negative charge displacement intensity. Variable, therefore, of δ^- = 0.340 a.u. negative charge, passing through the absence of charge displacement, represented in the absence of black - for the green color of δ^+ = 0.340 a.u. positive charge. The magnitude of the electric dipole moment $|\vec{p}|$ total obtained was p = 4.9771 Debye, perpendicular to the main axis of the molecule, for sets basis CC-pVTZ. By the distribution of charge through the bio-inorganic molecule it is clear that the molecule has a polar-apolar-polar structure, Figure (2) and Table (1).

An analysis of the individual charge value of each atom of the molecule could be made, but here it was presented only according to Figure (2), due to the objective being to determine the polar-apolar-polar, the polar characteristic of the molecule, whose moment of dipole is practically perpendicular to the central axis of the molecule.

In Figure (2) the dipole moment is visualized 6-311G** (3df, 3pd) and CC-pVTZ in base sets, being represented by an arrow in dark blue color, with their respective values in Debye. This also presents the orientation axes x, y and z and the distribution of electric charges through the molecule.

In the set of bases used the CC-pTZV and 6-311** (3df, 3pd) present the same characteristic for the distribution of charges to the polar end with Carbon atom (negative charge) bound to the $-SiH_3$ radical and the two Lithium atoms. It is seen that Δδ = 0.680 a.u. of CC-pTZV and Δδ = 1.366 a.u. of 6-311 (3df, 3pd), this latter has a twice greater Δδ, Figure (2), although the dipole moments CC-pTZV are 3.69% larger, Table (1).

The main chain (backbone of the molecule) for the CC-pTZV base set has a small negative charge displacement for the Carbon atoms from the Hydrogen atoms attached to them. Therefore, with positive charge the Hydrogen atoms connected to the Carbon of the central chain. For the set of bases 6-311**(3df, 3pd) the carbon atoms of the main chain are presented with very small distribution of negative charge, coming from the Hydrogen linked to these neutrals, Figure (2).

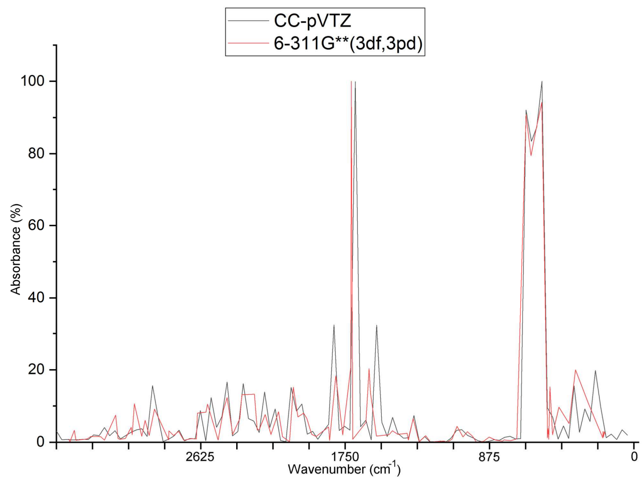

Figure 5. *Infrared spectrum obtained using the ab initio for the RHF [2-9] method, in sets of basis RHF/CC-pVTZ [10-14] in black color and 6-311G** (3df, 3pd) [7, 15-21] in red color, obtained using computer software GAMESS [15, 20]. Graphic edited in origin software, for comparison of the spectra obtained in the set of bases used. [72]*

At the other polar end for the base set 6-311** (3df, 3pd) the cyclic chain shows the characteristics as the Beryllium atom with strong charge displacement positive, these charges shift to the Carbon atoms attached to it, Figure (2). The cyclic chain with a strong negative charge, displaced from the Beryllium atom. The two carbon atoms bonded in double bonds, present a slight positive charge, with their neutral Hydrogen, Figure (2).The Selenium atom connected to two Carbon atoms of the cyclic chain presents a slight negative charge, originating from the Carbon atom connected to the main chain with a slight positive charge, and the other Carbon atom connected to the cyclic chain presents a neutral charge, Figure (2). The magnitude of the electric dipole moment $|\vec{p}|$ total obtained was p = 4.7936 Debye for 6-311** (3df, 3pd), Table (1).

Figures (3) and (4) represent the normalized infrared spectrum for the base set RHF / 6-311G ** (3df, 3pd) and CC-pVTZ for Absorbance and Transmittance.

Figures (5) represent the normalized infrared spectrum for the base set RHF/6-311G** (3df, 3pd) and CC-pVTZ for absorbance, making a comparison between the two sets of base.

The infrared spectrum for Standard RHF/CC-pVTZ shows peaks in transmittance, at wavelengths 1,125.44 cm^{-1}, 1,940.70 cm^{-1}, 2,094.82 cm^{-1}, 2,178.43 cm^{-1}, 2,613.99 cm^{-1} and transmittance 433.399 km/mol, 399.425 km/mol, 361.825 km/mol, 378.993 km/mol, 433.774 km/mol, respectively, Figure (3) and Table (2).

The infrared spectrum for Standard RHF/6-311G**(3df, 3pd) shows peaks in transmittance, at wavelengths 1,114.83 cm^{-1}, 1,936.81 cm^{-1}, 2,081.49 cm^{-1}, 2,163.23 cm^{-1}, 2,595.24 cm^{-1} and transmittance 434.556 km/mol, 394.430 km/mol, 345.287 km/mol, 375.381 km/mol, 409.232 km/mol, respectively, Figure (4) and Table (3).

It presents "fingerprint" between the intervals (680 cm^{-1} and 1,500 cm^{-1}) and (3,250 cm^{-1} and 3,500 cm^{-1}), Figures (3) (4) and (5).

5. Conclusions

Calculations obtained in the ab initio RHF method, on the set of basis 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 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 $C_{13}H_{20}BeLi_2SeSi$, for absorbance and transmittance, in Hartree method in the set of bases CC-pVTZ and 6-311G (3df, 3pd)

The infrared spectrum for Standard RHF/CC-pVTZ shows peaks in transmittance, at wavelengths 1,125.44 cm^{-1}, 1,940.70 cm^{-1}, 2,094.82 cm^{-1}, 2,178.43 cm^{-1}, 2,613.99 cm^{-1} and transmittance 433.399 km/mol, 399.425 km/mol, 361.825 km/mol, 378.993 km/mol, 433.774 km/mol, respectively.

The infrared spectrum for Standard RHF/6-311G**(3df, 3pd) [7, 30, 60, 71, 83, 84, 85, 86] shows peaks in transmittance, at wavelengths 1,114.83 cm^{-1}, 1,936.81 cm^{-1}, 2,081.49 cm^{-1}, 2,163.23 cm^{-1}, 2,595.24 cm^{-1} and transmittance 434.556 km/mol, 394.430 km/mol, 345.287 km/mol, 375.381 km/mol, 409.232 km/mol, respectively.

It presents "fingerprint" between the intervals (680 cm^{-1} and 1,500 cm^{-1}) and (3,250 cm^{-1} and 3,500 cm^{-1}).

The dipole moments CC-pTZV are 3.69% bigger than 6-311G (3df, 3pd).

As the bio-inorganic molecule $C_{13}H_{20}BeLi_2SeSi$ is the basis for a new creation of a bio-membrane, later calculations that challenge the current concepts of biomembrane should advance to such a purpose.

Acknowledgements

To the doctors: Prof. Ph.D. Tolga Yarman, Okan University, Akfirat, Istanbul, Turkey & Savronik, Organize Sanayi Bolgesi, Eskisehir, Turkey, and Prof. Ph.D. Ozan Yarman, Istanbul University, Rihtim Nr:1, 81300 Kadikoy, Istanbul, Turkey, for their valuable contributions to the work.

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