Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR) Spectroscopy Study of the Nano Molecule C_{13}H_{20}BeLi_{2}SeSi Using \textit{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_{2}SeSi. Calculations obtained in the \textit{ab initio} restrict Hartree-Fock method, on the basis set was used to indicate that the simulated molecule C_{13}H_{20}BeLi_{2}SeSi 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_{2}SeSi is of 15.799 Å. The ATR-FTIR spectrum was calculated for indicating the characteristic of the nano molecule and their frequency (cm\textsuperscript{-1}) were obtained in the basis set was used. The highest for ATR-FTIR scattering activities peaks are in the frequency 3.348 (cm\textsuperscript{-1}) with 7.107609729 (Å\textsuperscript{3}/amu) and 2.163 (cm\textsuperscript{-1}) with 8.902805583 (Å\textsuperscript{3}/amu) for RHF/CC-pVTZ and RHF/6-311G** (3df, 3pd), respectively. As the bio-inorganic molecule C_{13}H_{20}BeLi_{2}SeSi 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_{2}SeSi, 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_{2}SeSi. Calculations obtained in the \textit{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_{2}SeSi 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:

\[
\epsilon_{i}\psi_{i}(r) = \left(-\frac{1}{2}\nabla^{2} + V_{\text{ion}}(r)ight)\psi_{i}(r)\sum_{j}\int dr'\frac{|\psi_{i}(r')|^{2}}{|r-r'|}\psi_{j}(r) - \sum_{j}\delta_{\sigma'\sigma}\int dr'\frac{|\psi_{i}(r')\psi_{j}(r')|}{|r-r'|}\psi_{j}(r). \quad (1)
\]

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

\[
\text{HF} \ll \text{MP2} < \text{CISD} < \text{CCSD} < \text{CCSD (T)} < \text{FCI} \quad (2)
\]
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 model was used: Intel® Core™ i3-3220 CPU @ 3.3 GHz x 4 processors [65], Memory DDR3 4 GB, HD SATA WDC WD7500 AZEK-00RKA0 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 C13H20BeLi2SeSi molecule using the GAMESS [15, 20]. The set of programs GaussView 5.08 [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 C13H20BeLi2SeSi, 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 \textit{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 \textit{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$_{12}$H$_{20}$BeLi$_2$SeSi molecule via ab initio methods, basis set RHF/CC-pVTZ [66, 67, 68, 69, 70] for the ATR-FTIR spectrum.

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Table 2. Table containing the frequency (cm$^{-1}$) for intensity (km/mol) of the C$_{12}$H$_{20}$BeLi$_2$SeSi molecule via ab initio methods, basis set RHF/6-311G** (3df,3pd) for the ATR-FTIR spectrum.

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<th>$\nu$ (km/mol)</th>
<th>$\nu$ (cm$^{-1}$)</th>
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4. Discussions

The Figures (2-4) represent the ATR-FTIR spectrum of C_{13}H_{20}BeLi_{2}SeSi - 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, Å\(^4\)/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_{2}SeSi, 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_{2}SeSi, for absorbance and transmittance, in Hartree-Fock method in the basis set RHF/CC-pVTZ and 6-311G (3df, 3pd). The dipole moments CC-pVTZ 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 (Å⁴/amu) and 2,163 cm⁻¹ with 8.902805583 (Å⁴/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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