

A novel and exquisite approach to single layer bioinorganic membranes

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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 been 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 15.799 Å. 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 3,348 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. 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 characterizing 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 [1-100]

Results and discussion

Our results take place from the findings of the molecular dynamics of bio-inorganic nano-molecule $C_{13}H_{20}BeLi_2SeSi$. The results were summarized and shown in Figures 1 [1-100].

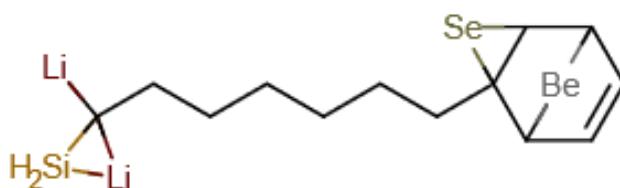


Figure 1. Representation of the molecular structure of $C_{13}H_{20}BeLi_2SeSi$, Nano-molecule Kurumi, 3-lithio-3-(6- {3-selena-8-beryllatricyclo [3.2.1.0^{2,4}]oct-6-en-2-yl}hexyl)-1-sila-2-lithacyclopropane, obtained through computer via *ab initio* calculation method RHF/CC-pVTZ [1-100]

Nano-Molecule Kurumi

The Figure 1 representation of the molecular structure of $C_{13}H_{20}BeLi_2SeSi$ / $C_{13}H_{19}BeLi_2SeSi$, 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 [1-100].

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