



Calculations Using Quantum Chemistry for Inorganic Molecule Simulation BeLi₂SeSi

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Abstract: Inorganic crystals have been used in the most diverse electronic systems since the nineteenth century, which apply to the wide variety of technological applications, which are the quartz crystals are the most used. Elements such as beryllium, lithium, silicon and selenium are widely used. The difficulty of finding such crystals from the combination of elements in nature or synthesized, suggest an advanced study of the same. In this sense, these elements were chosen because of the physical-chemical properties of each one, to simulate a seed molecule whose arrangement would be formed by the combination of these, aiming at the future development of a crystal to be used technologically. A study using computer programs with *ab initio* method was applied and the quantum chemistry was utilized through Molecular Mechanics, Hartree-Fock, Møller-Plesset and Density Functional Theory, on several bases. The main focus was to obtain a stable molecular structure acceptable to quantum chemistry. As a result of the likely molecular structure of the arrangement of a crystal was obtained, beyond the dipole moment, thermal energy, heat of vaporization and entropy of the molecule. The simulated molecule has a cationic molecular structure, in the atoms Selenium and Silicon. As a consequence, it has a strong electric dipole moment. Due to its geometry, it presents a probable formation structure of a crystal with a tetrahedral and hexahedral crystal structure.

Keywords: Beryllium, DFT, Lithium, Molecular Geometry, Selenium, Silicon

1. Introduction

A crystal [1] oscillator is an electronic oscillator circuit that uses the mechanical resonance of a vibrating crystal of piezoelectric material to create an electrical signal with a very precise frequency. This frequency is commonly used to keep track of time (as in quartz wristwatches), to provide a stable clock signal for digital integrated circuits, and to stabilize frequencies for radio transmitters and receivers. The most common type of piezoelectric resonator used is the quartz crystal, so oscillator circuits incorporating them became known as crystal oscillators, but other piezoelectric materials including polycrystalline ceramics are used in similar circuits. [2, 3]

The use of inorganic crystals technology has been widely date. Since quartz crystals [1] for watches in the nineteenth century, and common way radio in the early twentieth

century, to computer chips with new semiconductor materials. [2] Chemical elements such as beryllium, lithium, selenium and silicon, [1, 4] are widely used in technology. The development of new crystals arising from that arrangement can bring technological advances in several areas of knowledge.

Within many electronics resonates a crystal that determines a precise rhythm functioning. The clocks, timers, computers, communications equipment and many other tiny devices quartz crystals [1] vibrate accurately ensuring that your circuits work completely orderly and synchronized way. It is difficult to predict what would be electronics today without the presence of these elements. [5]

A study using computer programs with *ab initio* method was applied and the quantum chemistry was utilized through Molecular Mechanics, Hartree-Fock, Møller-Plesset and Density Functional Theory, on several bases. [6, 7]

A preliminary literature search did not indicate any compounds of said arrangement of these chemical elements. This fact the study can lead to getting new crystals to be used in the materials industry. A study using computer programs with ab initio have been applied. The calculations indicate by the ab initio methods used that the molecular structure of the simulated molecule can in more detailed calculations generate a crystalline structure. [8, 9]

2. Chemical Properties of the Compounds of Beryllium, Lithium, Selenium and Silicon

The Beryllium, Lithium, Selenium and Silicon elements were chosen due to their peculiar physicochemical properties and their wide use in industry and technology.

2.1. Beryllium

Beryllium is a chemical element with symbol Be and atomic number 4. It is created through stellar nucleosynthesis and is a relatively rare element in the universe. It is a divalent element which occurs naturally only in combination with other elements in minerals. Notable gemstones which contain beryllium include beryl (aquamarine, emerald) and chrysoberyl. As a free element it is a steel-gray, strong, lightweight and brittle alkaline earth metal. [2]

Beryllium improves many physical properties when added as an alloying element to aluminium, copper (notably the alloy beryllium copper), iron and nickel. [10] Tools made of beryllium copper alloys are strong and hard and do not create sparks when they strike a steel surface. In structural applications, the combination of high flexural rigidity, thermal stability, thermal conductivity and low density (1.85 times that of water) make beryllium metal a desirable

aerospace material for aircraft components, missiles, spacecraft, and satellites. [10] Because of its low density and atomic mass, beryllium is relatively transparent to X-rays and other forms of ionizing radiation; therefore, it is the most common window material for X-ray equipment and components of particle physics experiments [10]. The high thermal conductivities of beryllium and beryllium oxide have led to their use in thermal management applications.

2.2. Lithium

Lithium (from Greek: λίθος, *lithos*, “stone”) is a chemical element with symbol Li and atomic number 3. It is a soft, silver-white metal belonging to the alkali metal group of chemical elements. Under standard conditions it is the lightest metal and the least dense solid element. Like all alkali metals, lithium is highly reactive and flammable. For this reason, it is typically stored in mineral oil. When cut open, it exhibits a metallic luster, but contact with moist air corrodes the surface quickly to a dull silvery gray, then black tarnish. Because of its high reactivity, lithium never occurs freely in nature, and instead, only appears in compounds, which are usually ionic. Lithium occurs in a number of pegmatitic minerals, but due to its solubility as an ion, is present in ocean water and is commonly obtained from brines and clays. On a commercial scale, lithium is isolated electrolytically from a mixture of lithium chloride and potassium chloride. [2]

Lithium and its compounds have several industrial applications, including heat-resistant glass and ceramics, lithium grease lubricants, flux additives for iron, steel and aluminum production, lithium batteries and lithium-ion batteries. These uses consume more than three quarters of lithium production. [2]

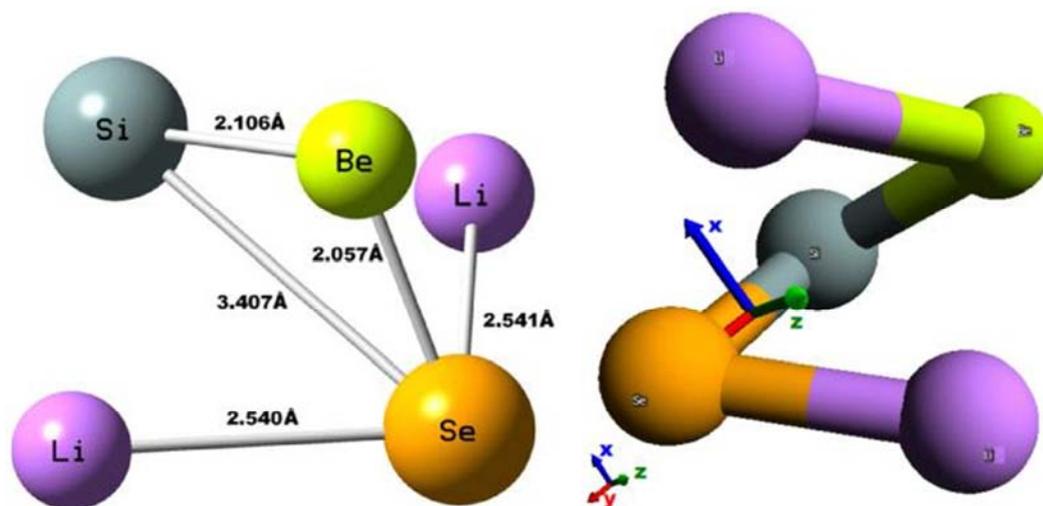


Figure 1. Above and to the left the representation of the molecular structure of BeLi_2SeSi seed [9], obtained through computer via Molecular Mechanics Mm+ calculation, and then its geometry was optimized via PM3 [12, 13, 14, 15, 16] with distance measured in Ångstrom obtained using computer programs Hyper Chem 7.5 Evaluation [6]. Above and to the right the representation of the molecular structure of BeLi_2SeSi , obtained through computer via Ab Initio calculation method DFT, functional B3LYP in base 6-311G**(3df, 3pd), obtained using computer programs GAMESS [7, 17]. Images obtained in the software Mercury 3.8 [18], above and to the left and the right Avogadro [19]. Represented in gray color the atom of Silicon, in the purple color Lithium, in the lemon yellow color Beryllium, and in the pumpkin the Selenium.

2.3. Selenium

Selenium is a chemical element with symbol Se and atomic number 34. It is a nonmetal with properties that are intermediate between those of its periodic table column-adjacent chalcogen elements sulfur and tellurium. It rarely occurs in its elemental state in nature, or as pure ore compounds. Selenium (Greek *selene* meaning “Moon”) was discovered in 1817 by J. Jacob Berzelius. [2]

Selenium is found impurely in metal sulfide ores, copper where it partially replaces the sulfur. The chief commercial uses for selenium today are in glassmaking and in pigments. Selenium is a semiconductor and is used in photocells. Uses in electronics, once important, have been mostly supplanted by silicon semiconductor devices. Selenium continues to be used in a few types of DC power surge protectors and one type of fluorescent quantum dot. [2]

2.4. Silicon

Silicon is a chemical element with symbol Si and atomic number 14. It is a tetravalent metalloid, more reactive than germanium, the metalloid directly below it in the table. [2] Is the eighth most common element in the universe by mass, but very rarely occurs as the pure free element in nature. It is most widely distributed in dusts, sands, planetoids, and planets as various forms of silicon dioxide (silica) or silicates. Over 90% of the Earth's crust is composed of silicate minerals, making silicon the second most abundant element in the Earth's crust (about 28% by mass) after oxygen. [11]

Elemental silicon also has a large impact on the modern world economy. Although most free silicon is used in the steel refining, aluminium-casting, and fine chemical industries (often to make fumed silica), the relatively small portion of very highly purified silicon that is used in semiconductor electronics (<10%) is perhaps even more critical. Because of wide use of silicon in integrated circuits, the basis of most computers, a great deal of modern technology depends on it. [2]

3. Methods

3.1. Hartree-Fock

The Hartree-Fock self-consistent method is based on the one-electron approximation in which the motion of each electron in the effective field of all the other electrons is governed by a one-particle Schrodinger equation. The Hartree-Fock approximation takes into account of the correlation arising due to the electrons of the same spin, however, the motion of the electrons of the opposite spin remains uncorrelated in this approximation. The methods beyond self-consistent field methods, which treat the phenomenon associated with the many-electron system properly, are known as the electron correlation methods. One of the approaches to electron correlation is the Møller-Plesset

(MP) perturbation theory in which the Hartree-Fock energy is improved by obtaining a perturbation expansion for the correlation energy. [20] However, MP calculations are not variational and can produce an energy value below the true energy. [21]

Another first principles approach to calculate the electronic structure for many-electron systems is the Density Functional Theory (DFT). In this theory, the exchange-correlation energy is expressed, at least formally, as a functional of the resulting electron density distribution, and the electronic states are solved for self-consistently as in the Hartree-Fock approximation. [22, 23, 24, 25] The Density Functional Theory is, in principle, exact but, in practice, both exchange and dynamic correlation effects are treated approximately. [26]

A hybrid exchange-correlation functional is usually constructed as a linear combination of the Hartree-Fock exact exchange functional,

$$E_X^{HF} = -\frac{1}{2} \sum_{i,j} \iint \Psi_i^*(\mathbf{r}_1) \Psi_j^*(\mathbf{r}_1) \frac{1}{r_{12}} \psi_i(\mathbf{r}_2) \psi_j(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 \quad (1)$$

and any number of exchange and correlation explicit density functionals. The parameters determining the weight of each individual functional are typically specified by fitting the functional's predictions to experimental or accurately calculated thermochemical data, although in the case of the “adiabatic connection functionals” the weights can be set a priori. [27]

3.2. B3LYP

The B3LYP (Becke, three-parameter, Lee-Yang-Parr) [28, 29] exchange-correlation functional is:

$$E_{XC}^{B3LYP} = E_X^{LDA} + a_0 (E_X^{HF} - E_X^{LDA}) + a_x (E_X^{GGA} - E_X^{LDA}) + E_C^{LDA} + a_c (E_C^{GGA} - E_C^{LDA}) \quad (2)$$

Are generalized gradient approximations: the Becke 88 exchange functional [30] and the correlation functional of Lee, Yang and Parr [31] for B3LYP, and E_C^{DA} is the VWN local-density approximation to the correlation functional. [32]

The three parameters defining B3LYP have been taken without modification from Becke's original fitting of the analogous B3PW91 functional to a set of atomization energies, ionization potentials, proton affinities, and total atomic energies. [33]

The first principles methods (i.e. HF and DFT) discussed above can be implemented with the aid of the GAMESS set of programs to study the electronic structure and to determine the various physical properties of many-electron systems. [7] A basis set is the mathematical description of the orbitals within a system (which in turn combine to approximate the total electronic wavefunction) used to perform the theoretical calculation. [34] 3-21G, 3-21G*, 6-31G, 6-31G*, 6-31G**, 6-311G, 6-311G*, 6-311G** are the basis sets used in the calculations. The functional Becke-style one parameter

functional using modified Perdew-Wang exchange and Perdew-Wang 91 correlation is used for DFT Calculations. [26, 35]

The SCF method and extensions to it are mathematically and physically considerably more complicated than the one-electron methods already discussed. Thus, one normally does not perform such calculations with pencil and paper, but rather with complicated computer programs. Terms like “Hartree–Fock”, or “correlation energy” have specific meanings and are pervasive in the literature. [36]

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



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. [37]

For calculations a cluster of 6 computer models was used: Prescott-256 Celeron D processors, [2] featuring double the L1 cache (16 KB) and L2 cache (256 KB), Socket 478 clock speeds of 2.13 GHz; Memory DDR2 PC4200 512MB; Hitachi HDS728080PLAT20 80 GB and CD-R.

The dynamic was held in Molecular Mechanics Force Field (Mm+), Eq. (1), after the quantum computation was optimized via PM3 and then by DFT, [21, 26] with functional B3LYP [38] and base 6-311G** [7, 21, 26]. The molecular dynamics at algorithm Polak-Ribiere [39], conjugate gradient, at the termination condition: RMS gradient [40] of 0, 1 kcal/A. mol or 405 maximum cycles in vacuum [6].

The first principles calculations have been performed to study the equilibrium configuration of BeLi₂SeSi molecule using the Hyperchem 7.5 Evaluation [41], Mercury 3.8 a general molecular and electronic structure processing program [18], Avogadro: an advanced semantic chemical editor, visualization, and analysis platform [19] and GAMESS is a computational chemistry software program and stands for General Atomic and Molecular Electronic Structure System [7] set of programs. The first principles approaches can be classified into two main categories: the Hartree-Fock approach and the density functional approach. [22]

4. Discussions

The BeLi₂SeSi molecular has:
 Chemical formula: BeLi₂SeSi
 Molecular mass: 130.93764 amu
 Crystal system: triclinic
 Density: 215.757 g/cm³
 Wyckoff sequence: a5

A covalent bonding structure between the atoms was initially suggested as shown in Figure (1). Selenium valences +6, Silicon +4, Beryllium +2 and Lithium +1 were considered as valences. Selenium binding to the silicon in triple bond, and this to Beryllium in simple bond. Two lithium and beryllium atoms and simple covalent bond to

Selenium.

The structure of the molecule was initially parameterized and made to the optimization of its geometry using Molecular Mechanics Mm+. [42] After optimization of the geometry via Mm+, it was optimized via PM3 [12, 13, 14, 15, 16], Figure (1), being the software used was the Hyper Chem 7.5 Evaluation [6]. Above the center and to the right of Figure (1), the molecular structure of the BeLi₂SeSi molecule was obtained by DFT [21] in the UB3LYP/6-311G**(3df, 3pd) using the GAMESS software. [7]

A detailed analysis of the molecular structure of the BeLi₂SeSi molecule was obtained using the GAMESS software [7]. We obtained the dipole moment and vibration frequencies of the BeLi₂SeSi molecule through ab initio calculations by the B3LYP, HF, MP2, CISD, CCSD, CCSD(T) and FCI methods [21], Tables (3) and (6).

We represent the BeLi₂SeSi molecule in this sequence of Figure (3) for a better understanding of its three-dimensional structure.

Figure (3) contains 16 images of the molecular structure of BeLi₂SeSi molecule in different positions under-rotation of the x and y axes. From the first image at the top left, a sequence of 16 images in turn sequence is displayed, from left to right and from top to bottom. The molecule is rotated in the x-direction from the first image until it returns to its initial position in the ninth image. From which you rotate y until you return to the starting position, last image in the lower right corner. The atoms are represented in four different colors. Silicon in golden color, Selenium in orange, Beryllium in lime-green and two lithium atoms in purple.

Analyzing Figures (1) and Figure (2) obtained by quantum chemistry by the *ab initio* method, we can see the structure of the simulated molecule. Making the necessary turns of visualization with the atom of Be in front of the screen, or the atom of Se, and centralizing these in a segment of line between them, Be and Se, these form a tetrahedron each. Six planes are formed, with six triangles belonging to these planes formed by the atoms, occupying its vertices: Be-Si-Li₂, Be-Si-Li₁ and Be-Li₁-Li₂ for the tetrahedron of the atom Beryllium, and Se-Si-Li₁, Se-Si-Li₂ and Se-Li₁-Li₂ to the tetrahedron of the Selenium atom. Both tetrahedrons connected to the same base, formed by the plane, with the atoms Si-Li₁-Li₂, as vertices of the base triangle of these.

The covalent bonds between the atoms of the simulated molecule have now changed with the covalent bonding sequence Li₂-Be-Si-Se-Li₁, i.e. Li-Be-Si-Se-Li, Figure (2), (in the center and the left).

In Tables (1) and (2) the pdb files of the simulated molecule are displayed. The Table (1) the pdb file of the molecular structure of molecule BeLi₂SeSi, obtained through computer via ab initio calculation method HF in base STO-3G [43, 44], obtained using computer programs Hyper Chem 7.5 Evaluation [6]. The Table (2) the pdb file of the molecular structure of molecule BeLi₂SeSi, obtained through computer via ab initio calculation method B3LYP in base 6-

311G**(3df, 3pd), obtained using computer programs GAMESS [7].

The Table (3) presents some thermochemical properties of the simulated molecule, such as: thermal energy, vaporization heat and molar entropy. All values obtained after a end optimization of the molecular geometry, using the DFT method, with B3LYP functional and base 6-311G** (3df, 3pd). The thermochemical values for the HF, MP2, CISD, CCSD(T), CC, CID and CI methods were calculated at the end geometry point B3LYP/6-311G**(3df, 3pd). [21]

The lowest and highest thermal energy obtained were 7,622 kcal/mol and 8,560 kcal/mol in the HF/3-21G and MP2/STO-3G methods, respectively.

The lowest and highest heat of vaporization were 18.592 kcal/mol.K and 20.718 kcal/mol.K in the HF/3-21G and B3LYP/6-311G** (3df, 3pd) methods, respectively.

The lowest and highest molar entropy obtained were 80.298 kcal/mol.K and 84.426 kcal/mol.K, in the HF/6-311G** (3df, 3pd) and CIS-FC/CC-PVDZ methods, respectively.

The Tables (4) and (5) present the parameters of the molecular geometry of the simulated molecule, such as spatial coordinates, length of the bonds between the atoms, angles and dihedral. The Table (1) shows the values for the dynamics via the HF method in the STO-3G base and Table (2) for the DFT method, functional B3LYP in base 6-311G**(3df, 3pd).

The Figures (1) and (2), to the left of these, the representation of the molecular structure of BeLi₂SeSi seed [8, 9, 45, 46], obtained through computer via Molecular Mechanics Mm+ calculation, and then its geometry was optimized via PM3 [12, 13, 14, 15, 16] and the representation of the molecular structure of BeLi₂SeSi seed, obtained through computer via *ab initio* calculation method HF in base STO-3G [43, 44], with distance measured in Ångstron and loads obtained using computer programs Hyper Chem 7.5 Evaluation [6], respectively.

There is a reduction of the average distance between atoms of the simulated molecule.

Through the calculations presented in Table (6) show that the lowest and highest electric dipole moment, have the values 0.9869 Debye and 8.9298 Debye, in the B3LYP/STO-3G and UHF/TVZ methods, respectively.

5. Conclusions

As a result of the likely molecular structure of the arrangement of a crystal was obtained. The techniques of

micro-crushing and conoscopic [47] analysis can lead to evidence and obtaining such crystals.

Calculations using quantum chemistry admit inorganic molecule BeLi₂SeSi.

As a result of calculations *ab initio* the molecular structure with a feature proposed by the simulated seed molecule, it is likely by quantum chemistry that a crystal structure of the arrangement can be obtained.

The simulated molecule has a cationic molecular structure, in the atoms Selenium and Silicon. As a consequence, it has a strong electric dipole moment, 8.9298 Debye, in UHF/TVZ methods. Due to its geometry, it presents a probable formation structure of a crystal with the tetrahedral and hexahedral crystal structure.

6. Tables and Figures

Table 1. Description of the .pdb file of the molecular structure of molecule BeLi₂SeSi, obtained through computer via *ab initio* calculation method HF in base STO-3G [43, 44], obtained using computer programs Hyper Chem 7.5 Evaluation [6].

HETATM	1	Si	1	-0.892	1.300	0.917
HETATM	2	Se	2	-0.010	-1.387	-0.224
HETATM	3	Be	3	-1.646	-0.283	-0.066
HETATM	4	Li	4	0.494	0.829	-0.850
HETATM	5	Li	5	-0.199	-0.606	1.992
CONNECT	1	2	3			
CONNECT	2	1	3	4	5	
CONNECT	3	1	2			
CONNECT	4	2				
CONNECT	5	2				
END						

Table 2. Description of the .pdb file of the molecular structure of molecule BeLi₂SeSi, obtained through computer via *ab initio* calculation method B3LYP in base 6-311G**(3df, 3pd), obtained using computer programs GAMESS [7].

HETATM	1	Se	1	0.883	-0.055	0.000
HETATM	2	Li	2	-0.319	1.382	-1.484
HETATM	3	Si	3	-1.359	-0.805	0.000
HETATM	4	Li	4	-0.319	1.382	1.484
HETATM	5	Be	5	-2.273	1.212	0.000
CONNECT	1	2	3			
CONNECT	2	1				
CONNECT	3	1	5			
CONNECT	4	5				
CONNECT	5	3	4			
END						

Table 3. Thermochemical parameters of the molecule BeLi₂SeSi obtained by *ab initio* methods.

Methods/Base	Thermochemistry		
	E ^T Thermal (Kcal/mol)	CV (cal/mol.K)	S (cal/mol.K)
B3LYP/6-311G**(3df, 3pd)	8.152	20.718	83.606
CIS-FC/CC-pVDZ	8.523	19.714	80.298
HF/3-21G	7.622	18.592	82.660
HF/6-311G**(3df, 3pd)	8.158	20.706	84.426

Methods/Base	Thermochemistry		
	E _{Thermal}	CV	S
	(Kcal/mol)	(cal/mol.K)	(cal/mol.K)
MP2/STO-3G	8.560	19.648	80.457
CISD/STO-3G	8.552	19.662	80.457
CCSD(T)/STO-3G	8.518	19.749	80.714
CI/STO-3G	8.552	19.662	80.457
B3LYP/STO-3G	8.438	19.944	80.979
CC/STO-3G	8.545	19.686	80.609
CID/STO-3G	8.560	19.645	80.445

Table 4. Molecular parameters of the atoms of the molecule BeLi₂SeSi seed, obtained through computer via ab initio calculation method HF in base STO-3G [43, 44], with distance measured in Ångstron obtained using computer programs Hyper Chem 7.5 Evaluation [6].

Atom	NA	NB	NC	Bond	Angle	Dihedral	X(A) [°]	Y(A) [°]	Z(A) [°]
Si							-0,379	-1,080	1,707
Se	1			3,0272777			-0,671	0,681	-0,738
Be	2	1		1,8506712	40,6512698		-1,661	-0,539	0,240
Li	1	3	2	2,4351417	69,0527075	53,4172985	-0,624	1,341	1,614
Li	3	2	1	2,4492640	68,7308859	-58,1835086	0,412	-1,542	-0,594

Table 5. Molecular parameters of the atoms of the molecule BeLi₂SeSi seed, obtained through computer via ab initio calculation method DFT, functional B3LYP in base 6-311G**(3df, 3pd), with distance measured in Ångstron obtained using computer programs GAMESS. [7].

Atom	NA	NB	NC	Bond	Angle	Dihedral	X(A) [°]	Y(A) [°]	Z(A) [°]
Se							0.883497	-0.054990	0.000003
Li	1			2.390969			-0.319339	1.382430	-1.484498
Si	1	2		2.364837	73.358		-1.359205	-0.805152	-0.000012
Li	1	3	4	2.390972	73.357	40.393	-0.319392	1.382375	1.484518
Be	3	3	2	2.214531	95.889	-40.393	-2.273460	1.211847	0.000006

Table 6. Table containing the dipole moments of the BeLi₂SeSi molecule via ab initio methods.

Methods/Base	Dipole moment (Debye)			
	X	Y	Z	Total
UHF/CC-PVQZ [48, 49, 50, 51, 52]	0.8228	4.3880	0.0000	4.4645
UHF/CEP-31G [53, 54, 55]	0.7997	5.2102	0.0002	5.2712
UHF/CEP-121G [53, 54, 55]	0.7864	5.3204	0.0001	5.3782
UHF/SDD [56, 57]	-0.8772	6.8195	0.0000	6.8757
SDD All [56, 57]	0.5963	5.4523	0.0001	5.4848
UHF/SDD Ar/STO-3G [43, 44, 56, 57]	-1.3862	0.7216	0.0000	1.5627
UHF/SDF [56, 57]	0.6394	5.3161	0.0003	5.3544
UHF/UGBS1P [58, 59, 60, 61, 62, 63, 64, 65, 66]	0.5085	4.6007	0.0002	4.6287
UCISD-FC/STO-3G [43, 44, 67, 68, 69]	-0.8474	-0.9167	0.0022	1.2484
UHF/CEP-4G [53, 54, 55]	-0.1523	3.8818	0.0000	3.8848
UHF/CEP-31G [53, 54, 55]	-1.2259	5.1166	0.0000	5.2614
UHF/CEP-121G [53, 54, 55]	-1.1199	5.0853	0.0000	5.2071
UHF/LanL2MB [43, 44, 70, 71, 72]	-2.5964	5.5830	-0.2414	6.1620
UHF/LanL2DZ [56, 70, 71, 72]	-1.3022	4.3037	-0.1042	4.4976
UHF/LanL2MB/STO-3G [43, 44, 70, 71, 72]	-1.6159	0.5603	-0.0001	1.7103
LanL2DZ [43, 44, 70, 71, 72]	-1.3022	4.3037	-0.1042	4.4976
UHF/SDD † [56, 57]	-1.8520	5.9664	0.0000	6.2472
UHF/SDDAII [56, 57]	-1.1776	5.0344	0.0000	5.1703
UHF/CC-PVTZ [48, 49, 50, 51, 52]	-0.4389	5.0838	0.0000	5.1028
UHF/CC-PVQZ [48, 49, 50, 51, 52]	-0.4379	5.1418	0.0000	5.1604
UHF/SV [73, 74]	-1.3423	8.3589	0.0000	8.4660
UHF/TVZ [73, 74]	-1.4678	8.8083	0.0000	8.9298
UHF/STO-3G [7, 25, 39, 56, 75, 76, 77, 78]	-1.3862	0.7216	0.0000	1.5627
UBLYP/STO-3G [7, 25, 39, 56, 75, 76, 77, 78]	-0.4887	-1.0666	-0.0001	1.1732
UB3LYP/STO-3G [7, 25, 39, 56, 75, 76, 77, 78]	0.8327	-0.6992	0.0000	1.0873
UB3LYP/3-21G [7, 25, 39, 56, 75, 76, 77, 78]	-0.0682	4.6195	0.0000	4.6200
UB3LYP/6-31G(d) [7, 25, 39, 56, 75, 76, 77, 78]	0.2063	4.0714	0.0000	4.0766
UB3LYP/6-31G [7, 25, 39, 56, 75, 76, 77, 78]	-0.0435	4.9571	0.0000	4.9573
UB3LYP/6-311G [7, 25, 39, 56, 75, 76, 77, 78]	-0.4081	4.6962	0.0000	4.7139
UB3LYP/6-311G(d) [7, 25, 39, 56, 75, 76, 77, 78]	0.0271	4.0669	0.0000	4.0670
UB3LYP/6-311G(3df, 3pd) [7, 25, 39, 56, 75, 76, 77, 78]	0.1373	3.9598	0.0000	3.9622
UB3LYP/6-311G(d, p) [7, 25, 39, 56, 75, 76, 77, 78]	0.0271	4.0669	0.0000	4.0670
UB3LYP/6-311G**(3df, 3pd) [7, 25, 39, 56, 75, 76, 77, 78]	0.1374	3.9526	0.6081	4.0015

Methods/Base	Dipole moment (Debye)			
	X	Y	Z	Total
UCIS-FC/CC-PVDZ [48, 49, 50, 51, 52, 79]	-0.5403	5.0436	0.0000	5.0724
UHF/3-21G [7, 25, 39, 56, 75, 76, 77, 78]	-0.8811	4.9453	0.0000	5.0232
UHF/6-311G**(3df, 3pd) [7, 25, 39, 56, 75, 76, 77, 78]	-0.4440	5.1327	0.0000	5.1519
UMP2-FC/STO-3G [43, 44, 80, 81, 82, 83, 84, 85]	-1.6159	0.5603	-0.0001	1.7103
UCCSD(T)-FC/STO-3G [43, 44, 86, 87, 88, 89, 90, 91]	-1.6152	0.5864	0.0181	1.7185
UCISD-FC/STO-3G [43, 44, 92, 93, 94]	-0.8474	-0.9167	0.0022	1.2484
B3LYP/STO-3G [7, 25, 39, 43, 44, 56, 75, 76, 77, 78]	-0.7344	-0.6592	-0.0001	0.9869
UCCD-FC/STO-3G [43, 44, 86, 87]	-0.7643	-1.1334	0.0022	1.3670
UCID-FC/STO-3G [43, 44, 92, 93, 94]	-0.8846	-0.8808	0.0022	1.2483

† D95 up to Ar [56] and Stuttgart/Dresden ECPs on the remainder of the periodic table. [57] Selects Stuttgart potentials for $Z > 2$.

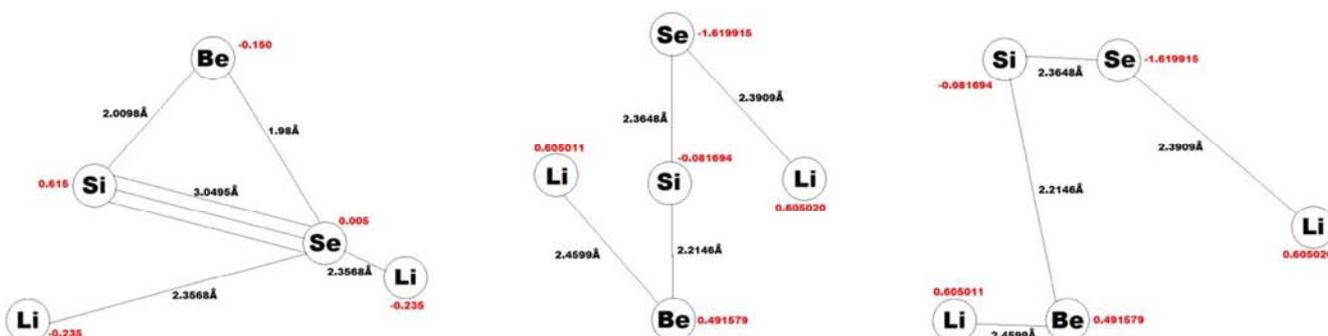


Figure 2. Above and to the left the representation of the molecular structure of BeLi_2SeSi seed, obtained through computer via *ab initio* calculation method HF in base STO-3G [43, 44], with distance measured in Ångstrom and loads obtained using computer programs Hyper Chem 7.5 Evaluation [6], after the structure of the molecule was initially parameterized and made to the optimization of its geometry using Molecular Mechanics Mm^+ . [42] After optimization of the geometry via Mm^+ , it was optimized via PM3 [12, 13, 14, 15, 16], Figure (1). Above, in the center and to the right the representation of the molecular structure of BeLi_2SeSi , [18] obtained through computer via *ab initio* calculation method DFT [21], functional B3LYP in base 6-311G**(3df, 3pd), with distance measured in Ångstrom and loads in units of atomic charge obtained using computer programs GAMESS [7].

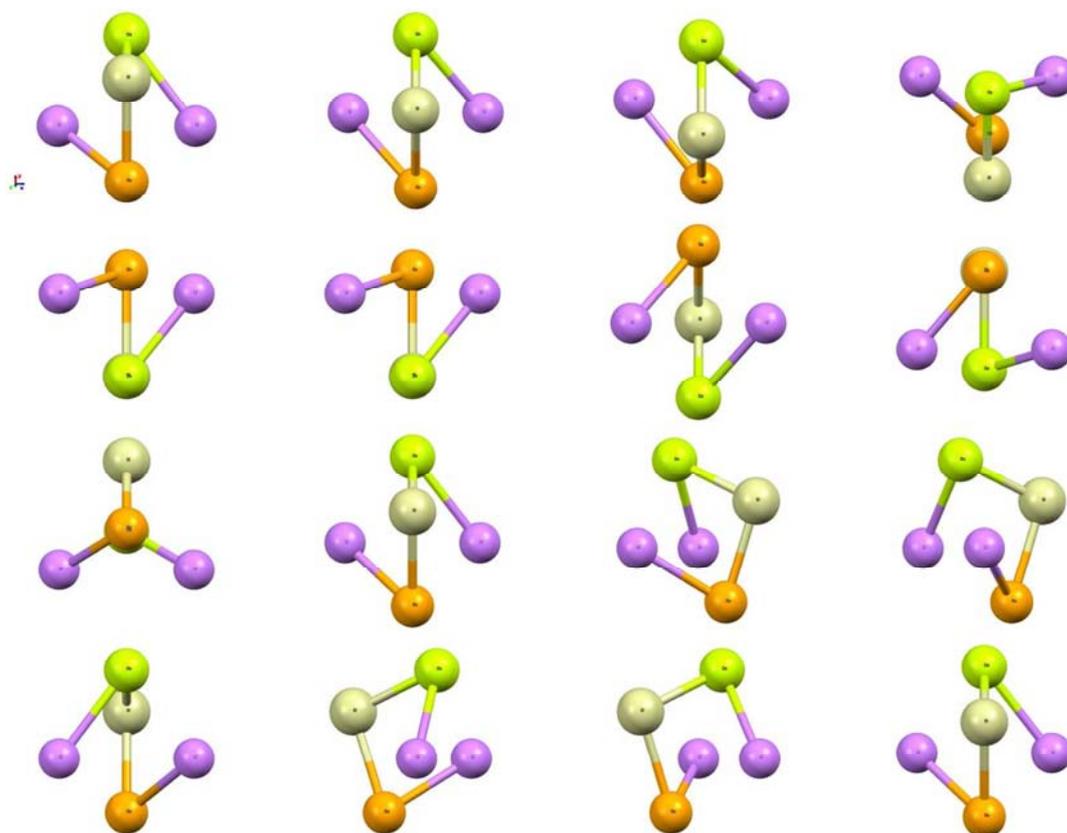


Figure 3. Representation of the molecular structure of BeLi_2SeSi , [18] obtained through computer via *ab initio* calculation method DFT, functional B3LYP in base 6-311G**(3df, 3pd), obtained using computer software GAMESS [7]. Images obtained in the software Mercury 3.8 [18]. Represented in cornsilk color the atom of Silicon, in the purple color Lithium, in the lemon yellow color Beryllium, and in the pumpkin the Selenium.

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