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STUDY OF THE SPECTRAL PROPERTIES OF THE DISELENIUM DICHLORIDE (Se_2Cl_2) MOLECULE IN THE I. R. INFRARED AREA

Hadeer Mohammed Farhan 1,
Ahmed Mohammed Farhan 2
Dakhil A. Abdzaid 3
1,3Ministry of Education, Alqadisiyah, Iraq
1University of Al-Qadisiyah, College of Biotechnology, Alqadisiyah, Iraq
1hadeern962@gmail.com ,2ahmed.mohammed@qu.edu.iq and 3d.abbas3344@gmail.com

Abstract:

The spectral and thermal properties of (Selenium-Halogen (Se2Cl2)) have been studied in this study, where the spatial geometry of the particles was studied using semi-experimental quantum programs in methdd (MNDO/PM3) via the dimensions of bonds. The basic molecule vibration frequencies, which have six basic vibration frequencies ranging from (69.34 - 456.01) cm-1 in the chair-form state, were also measured. The power is equal to (E.A = 2.047253eV), (Eg = 1.655715eV) and the distance quantity was determined to measure electronic affinity (E.A). The energy levels were then represented by two-dimensional (2D) and three-dimensional (3D) diagrams, and the total particle charge density and electrostatic voltage were determined using the HYPERCHEM software for most of the previous readings.

Keyword: Spectral, Selenium, Halogen, HYPERCHEM 6, MNDO / pm3, molecular orbitals.

Introduction

دراسة الخصائص الطيفية لجزيئة ثاني كلوريد الديسيلينيوم (Se2Cl2) في منطقة الأشعة تحت الحمراء (I.R.)

هدير محمد فرحان[1] , احمد محمد فرحان[2] , داخل عباس عبد زيد[3]
وزارة التربية/مديرية تربية القادسية[1,3] ،وزارة التعليم العالي والبحث العلمي/ جامعة القادسية / كلية العلوم[2]

الملخص:

في هذه الدراسة، تمت دراسة الخصائص الطيفية والحرارية لمركب (سيلينيوم-هالوجين (Se2Cl2)) حيث تم تحليل الهندسة الفراغية للجزيئات باستخدام برامج كمومية شبه تجريبية بطريقة (MNDO/PM3) من خلال أبعاد الروابط. كما تم قياس ترددات الاهتزاز الأساسية للجزيء، والتي تتضمن ستة ترددات اهتزاز أساسية تتراوح بين (69.34 - 456.01) سم-1 في حالة الشكل الكرسي (chair-form). وتساوي القدرة (E.A = 2.047253eV)، كما تم (Eg = 1.655715eV)،

European Science Methodical Journal
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تحديد كمية المسافة لقياس الألفة الإلكترونية (Electronic Affinity - E.A). بعد ذلك تم تمثيل ، كما تم تحديد كثافة الشحنة (Dوثلاثية الأبعاد (3 (Dمستويات الطاقة بواسطة مخططات ثنائية الأبعاد (2 الكلية للجزيء وجهد الكهرباء الساكنة باستخدام برنامج HYPERCHEM لمعظم القراءات السابقة.

الكلمات المفتاحية: طيفي (Spectral)، سيلينيوم(Selenium)، هالوجين(Halogen)6، هايبركيم (Molecular Orbitals)، المدارات الجزيئية(MNDO / pm3)، إم إن دي أو / بي إم 3(HYPERCHEM 6)

Introduction

The study of the interaction of electromagnetic waves with matter can be known as the molecular spectrum. Since this spectrum will provide us with details about the molecular structure of matter and that when we need a high-power analyzer, the molecular spectrum occurs in the form of large bands (this is what separates it from the atomic spectrum), where a group of spectral lines arising from a number of transitions [1,2,3]. Depending on the frequency or wavelength, the electromagnetic spectrum consists of several regions, beginning with radio waves and ending with gamma rays and cosmic rays. The following fields are composed of:

A- The gamma ray region (γ-rays) and its frequency is greater than 3×10^{19} Hz (with a wavelength (0.1-1A °) and the beam causes nuclear alterations. The region of frequencies confined between (3×10^{18}-3×10^{16})Hz represents the region of x-rays , and the spectral changes include the internal electrons of the molecules. Energies greater than (10^{7} J / mole), that is, more than (10 eV).

B- The visible and ultraviolet rays region extending to the frequencies confined between (3.75×10^{14}Hz to 1.5×10^{16}Hz), and it includes electronic transitions of valence electrons from one molecular orbital to another. Energy in terms of wavelengths in units of inclines (1A ° = 10^{-8} cm).

C- The infrared region, which includes the confined frequency area Between 1.7×10^{14} Hz and 1×10^{12} (0.8-300) micrometers, it includes transitions between the vibrational energy levels of the molecule, and thus the type is called Vibrational spectroscopy(wave number) in units of cm^{-1}.

D- The microwave area includes the frequency range between 3×10^{11}Hz to 10^{9}Hz (i.e. 1mm-30cm) and includes transitions between levels.The spin energy of the molecule can also be studied in electron spin resonance spectroscopy . Radio waves are being analyzed in the micro-ray field of nuclear magnetic resonance spectroscopy. There are several kinds of energy states, as described earlier, and we will concentrate here on levels of rotational energy (F) and vibrational energy (G) only, as the rotational motion is typically followed by a vibrational motion as a result of the two nuclei vibrating relative to each other. The particle rotation spectrum is a measure of the transitions that occur in the allowable energy ranges, and in the micro-wave spectroscopy region and the far infrared region, the rotational transitions occur and are due to the transition from the microwave region. Pure rot.). To give the particle a rotating

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spectrum, if the transformation happens at energy levels, it must have an electric dipole moment on the other hand. Vibration (as a result of increasing the excitation energy), in addition to changes in the levels of rotation and this absorption or emission due to rotation, the emission would appear due to changes in the numbers of the vibrational quantum [1]. This region is divided into three main regions, which are regionFar infrared ray (Far I.R.) ranges between (10-200) cm $^{-1}$ and area.The middle infrared ray (Mid I.R.) and ranges between (200-4000) cm $^{-1}$ and the near infrared area (Near I.R.) and ranges between (4000-12000) cm -1.Figure (1) illustrates that [4,1]:

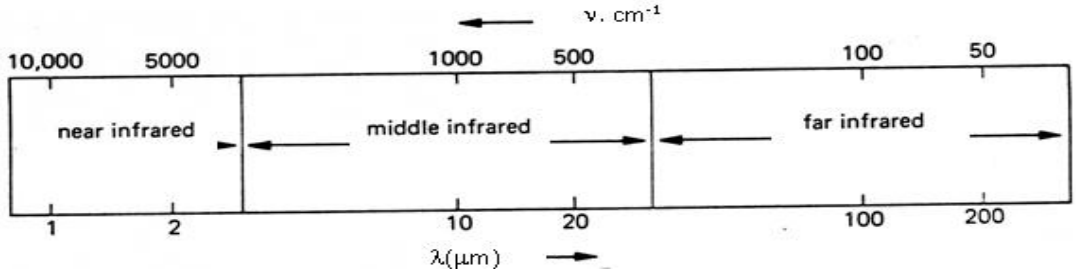

Figure (1) represents the main IR regions [4].

The middle infrared region is concerned with the study of pure vibrational transitions (pure -vib.)444 As well as rotational vibrational transitions (Rot-vib.trans.),Therefore the rotational spectra cannot be separated from the vibrational spectra [1]. The vibrational rotational spectra of polyatomic particles in the infrared region are more complex than the spectra of binary particles. Where there are differences in the selection rules and formulas for energy levels, and thus in the appearance of the spectral beam, the equation for calculating the rotational and vibrational energy is

$$T(J,V)=BJ(J+1)+(A-B)K^2+(V+\frac{1}{2})\omega-(V+\frac{1}{2})^2X_e\omega_e \quad ------(1)$$

$$J=0,\ 1,\ 2,.....,K=0,\ \pm1,\ \pm2,.....$$

And the linear particles have the following form:

A- Parallel vibration (||): The selection rules are as follows

$$\Delta J=\pm1, \qquad \Delta V=\pm1$$

It is therefore expected that the spectrum of a linear polyatomic molecule consists of two branches with a loss of spectral line at the center of the beam

B- Vertical vibration ((⊥)): The selection rules are as follows

$$\Delta J=0,\pm1\ , \quad \Delta V=\pm1$$

Thus, the vertical vibrating beams have branches where the spectral lines are located on top of each other in the center of the beam forming a high-intensity spectral line [2]. As for the symmetric top particles, they are:

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A- Parallel vibration (||). The selection rules are as follows

$$\Delta K = 0 \ , \quad \Delta V = \pm 1 \quad , \quad \Delta J = 0, \pm 1$$

Where a quantum number is equal to the low and high vibration levels, so the rotational frequencies do not depend on (k).

$$\Delta K = \pm 1 \ , \quad \Delta V = \pm 1 \quad , \quad \Delta J = 0, \pm 1$$

B- Vertical vibration ($\perp$): The selection rules are in the form

This means that the change of (K) gives branches as shown in the figure No. (1). As the greater the number of atoms in the molecule, the more complex the lines that are Evidence that the beam is vertical. The shape is nearly the same for linear and nonlinear particles, but the interactions are smaller and convergent for nonlinear particles, so it is difficult to analyze and only the Q-branching appears as a distinct line. The vertical vibrating beams have branches where the spectral lines lie on top of each other in the center of the beam forming a high-intensity spectral line [2]. As for the symmetric top particles, they are:

Evidence that the beam is vertical. The shape is nearly the same for linear and nonlinear particles, but the interactions are smaller and convergent for nonlinear particles, so it is difficult to analyze and only the Q-branching appears as a distinct line.

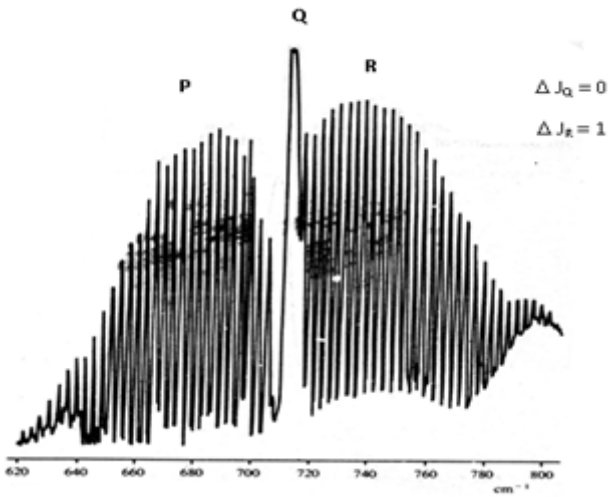

Figure (2) HCN particle vertical vibrational spectrum (bending) It shows branches[2]

There are beams whose intensity is weak relative to basic beams of weak impact.The incompatibility factor in it. It is caused by a decrease in the distance between energy levels Seismicity and the possibility of additional transitions (other than the fundamental frequency), which are:

1- Overton bands
2- Combination bands
3- Difference bands
4-Fermi & hot bands

Electron affinity:

is the energy that is released when an atom binds an electron to it. Such as items whose outer covers contain seven electrons (such as halogens) have the highest electronic affinity because they need an electron to reach a saturated outer shell.And when atoms combine to form molecules, there are two kinds of intertwining, bonds Pure ionic and other pure covalent. A pure ionic bond requires that an atom be completely lost to its electron (or more) and transferred (or transferred) to another atom or atoms that form ions. As for Pure covalent synergy requires that two (or more) electron atoms share equally. The parameter that is related to the degree of attraction of an atom in a compound to an electron is called electron negative. Mulliken was able to find the relationship to calculate the electrical negativity (Z) with ionization potential (I) and electronic affinity (A). As shown in the following relationship [5]

$$Z=\frac{I+A}{5.6} \quad -----(2)$$

Pauling was also able to calculate the electrical negativity values by using the energy difference (E) between the true pinion energy and the covalent bond energy, and he made this difference a measure of the electrical negative difference between the two pus atoms. Negativity helps Electrical to know the ionic property of the pinhole. The greater the difference in electrical negativity between the two atoms of the compound, the more ionic, i.e. more polar, the compound. Because of the mathematical difficulties arising from the application of quantum mechanics to particles, and the attempt to use experimental methods and concepts to describe interactions. Therefore, approximate methods were adopted to describe this interaction during the description of the molecular electronic structure using the molecular orbital method. And under dealing with the topic, the introduction of appropriate wave functions. In the cases of hybrid orbitals, for example, the molecular orbitals (σ) appear as stomata Which is due to the direct superposition of the atomic orbitalin. Whereas orbital (π) is when close to the orbitalan two atoms of type (P) and the axis of the orbitalin parallel to each other and perpendicular to the axis of the spurs between the two atoms. Molecules have shapes specific means the presence of a directional property of the bonds formed around an atom. It should be recognized that the covalent bonds can have a directional property and try to form orbitals Hybrids fit these trends. We often encounter an interference (direction) of one or three orbitals during crossbreeding. Associative molecular orbitals have a concentrated electron density between two nuclei and this state is an isotropic state, because the electron between the two nuclei is attracted to both. The foregoing shows the great importance of the emergence of Orbital theory of molecular

structure (Huckel-Molecular orbital theorem) and its abbreviation (HMO) were intended to relate the properties of unsaturated molecules. And how to apply them in basic approximations on some organic double molecules are interlinked The defining feature of this Molecules are the possibility to classify their valence electrons into two separate denominations Electrons (σ) (strongly concentrated in bonds and are relatively inactive),And the (pi) electrons (which are more effective and play a fundamental role in the chemical reactions of molecules. They are not concentrated, but rather moving over the carbonic structure of the molecule), for example, formaldehyde bold (the molecule under investigation). It is present on the carbon atom. To calculate the electrostatic voltage, we use the following equation [3]

$$V(r) = \sum_{A} \frac{Z_A}{|R_A - r|} - \int \frac{\rho(r)}{(\vec{r} - r)} d\vec{r} \quad \text{--------(3)}$$

Where it is after the positive charge and it is the nuclear charge of the atom A which is a distance away and the function represents the electronic density and represents the first term of the equation (3).The contribution of the cores to the electrostatic voltage, while the second term represents the electronic contribution [3].And during the HyperChem program you can view the electrostatic field.In the form of two-dimensional contour drawings (2D Contours) or three-dimensional stereoscopic graphics (3D Isosurface). You can also control the shape of these contours or figures, where we notice the contour map and the three-dimensional graphics in several levels and identify the shape of the charge distribution of the group, which is the goal of the research.

Diselenium dichloride:

is-an inorganic compound with the formula Se_2Cl_2. It is plotted as follows

Table(1): Some of properties of se2cl2 molecule(6)

Appearance	Density g/mL	Melting Point°C	Solubility
dark brown red liquid	2.73	-85	Soluble in chloroform, benzene, carbon tetrachloride, carbon disulfide;

As the number of atoms that make up the molecule (N = 4); Therefore, the number of degrees of freedom is (3N = 12) degrees and the number of vibrational patterns according to the rule (3N-6) for being a non-linear particle is (6) degrees where there are (3) degrees of rotational

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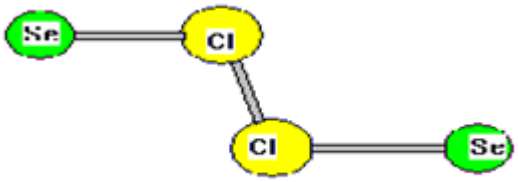
motion and (3) degrees of translational motion. The structural shape of the molecule was drawn from program (Hyper chem.), And is shown in Figure (3).



Figure(3): the shape of Se2cl2 draw using by Program Hyperchem

Results and discussion:

-Description of vibrational patterns

Using the program (Hyper chem.), The vibrational frequencies of the molecule are calculated in units of (cm^{-1}) with giving some other spectral characteristics such as: the intensity of each pattern in units of (km / mol), as well as the symmetry type for each of the patterns. Vibration of the molecule. Figure (2) represents one of the steps of the (Hyper chem.) Program, in which the basic vibration patterns are explained**.**

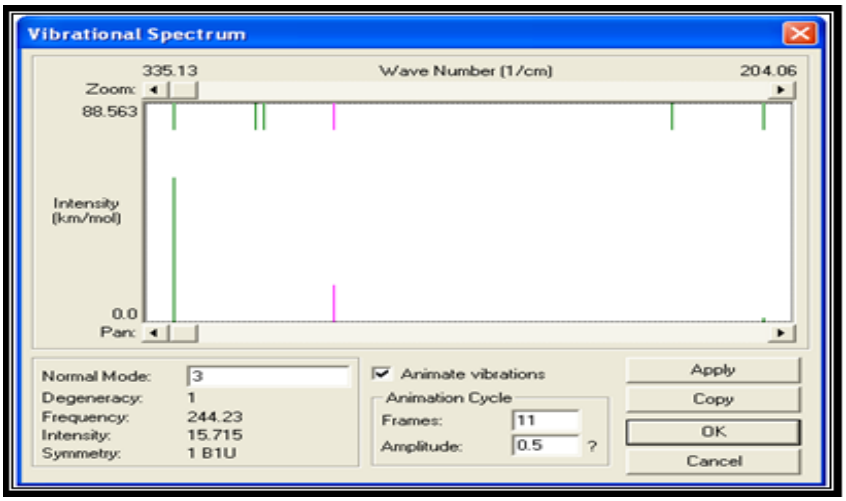


Figure (4) Hyper Chem program interface showing frequency, intensity, and symmetry

European Science Methodical Journal
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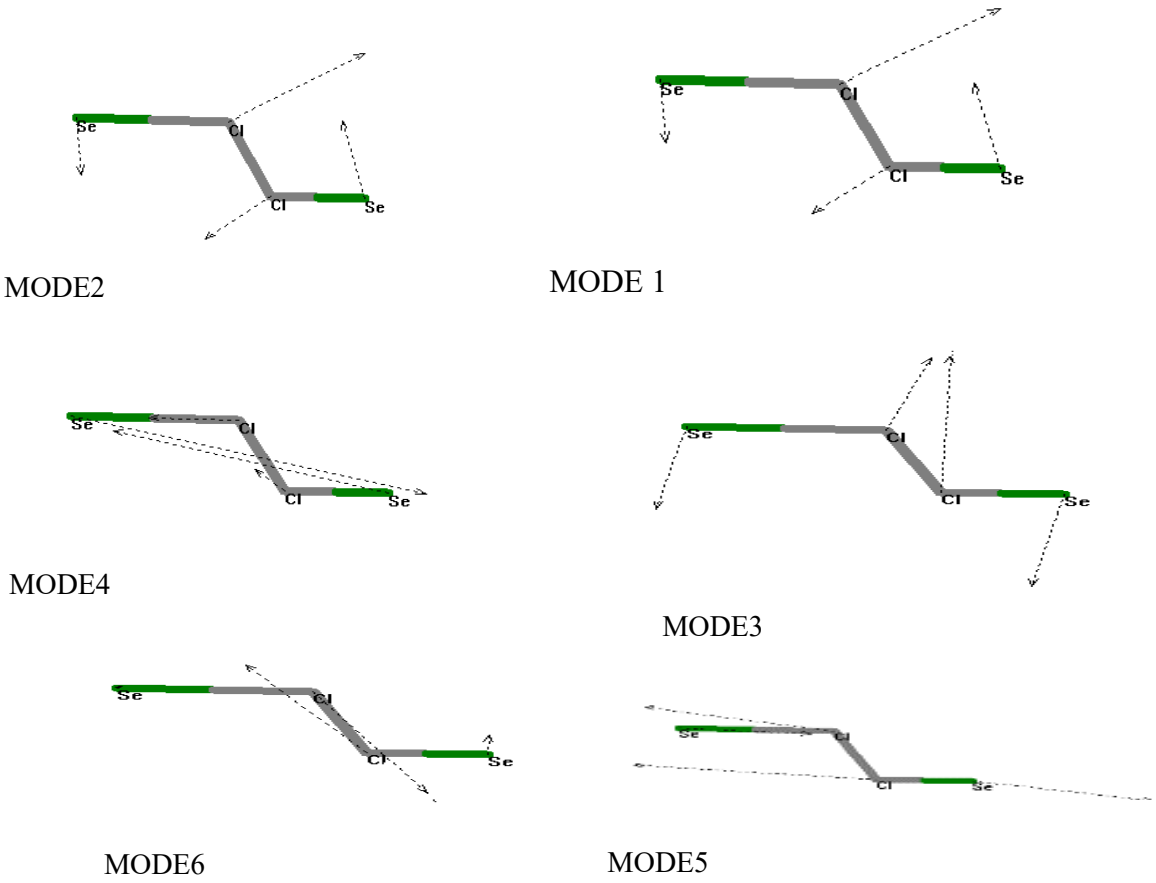
The following results were obtained for the six vibration patterns and are shown in the following table

Mode	Degenercy	Frequency cm^{-1}	Intensity Kcal/mol	Symmetry
1	2	69.34	0.962	1BU
2	2	69.64	0.094	1AU
3	1	108.00	0.000	1AG
4	1	417.11	0.000	2AG
5	1	432.11	12.670	2BU
6	1	456.01	0.001	3AG

Table(2): Some values specific to the molecule Se2cl2

In a further step within the same program, the six basic vibration patterns of the molecule according to the rule (3N-6) were described from the shapes and drawings of the particle, showing the directions of vibrational motion of the molecule with arrows, Fig. (5).



Figure(5): The shapes of the six vibrational patterns of the moleculeSe2Cl2

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From the table (2), we notice the intensity value for patterns 3 and 4 is equal to zero, and this is evidence that the two intensities are in opposite directions, one canceling the other, and this is what we notice in Fig. (5) for patterns 3 and 4.

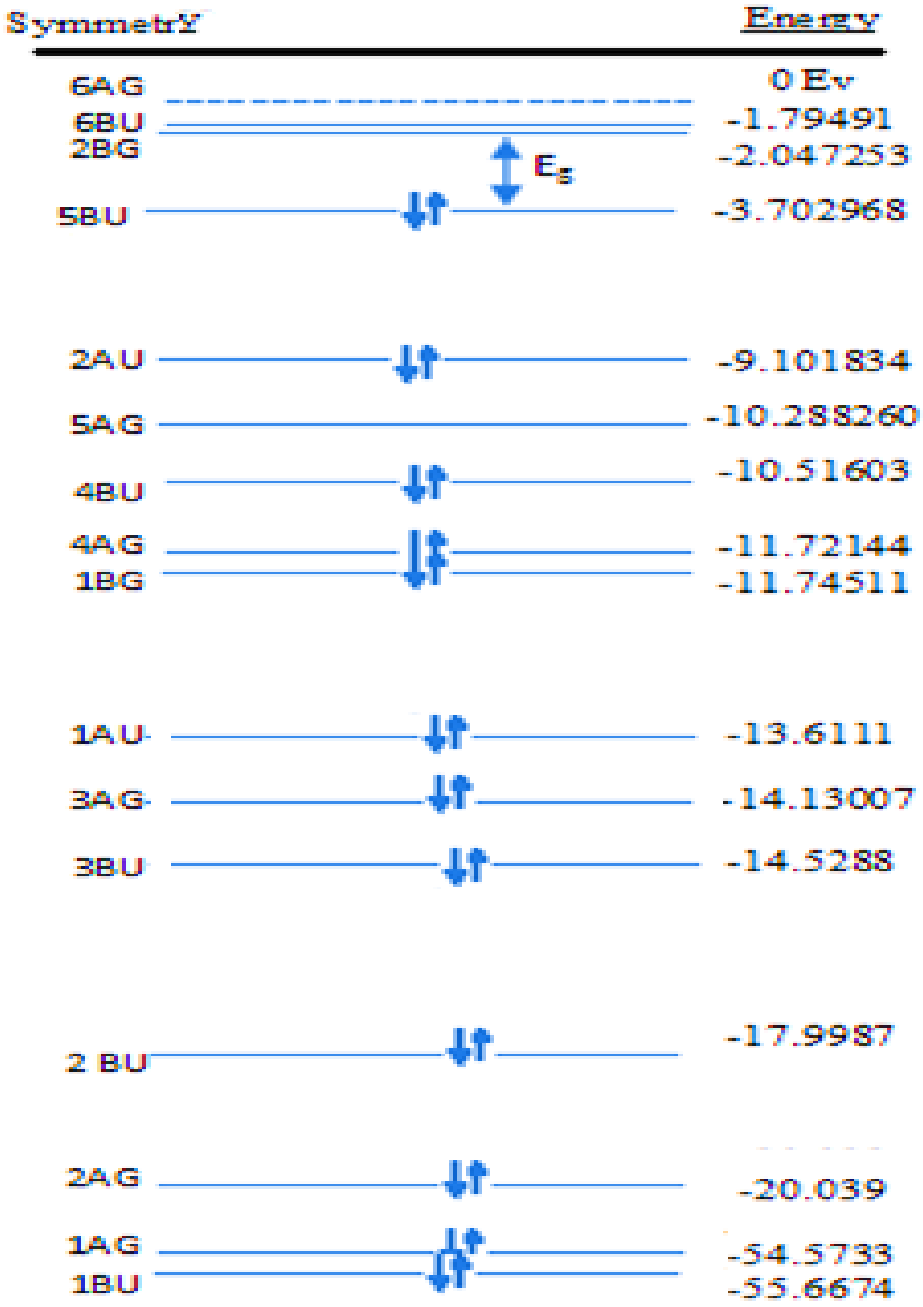

Figure (6): The molecular energy levels of (Se2Cl6) and the energy of (E_{HOMO} and (E_{LUMO})
The Ionization potential of the molecule was calculated , symbolized by (I.P), and its value was (I.P = 3.702968eV), The energy gap of the molecule was calculated(E_g =1.655715 eV), Through the value of the energy gap it is clear that the molecule is a semiconductor[7].

Conclusions:

1- The molecule is not linear and is subject to the 3N-6 relationship to know the number of vibrational patterns and their number is six

2- Through the results and tables, we notice that the intensity values for some values are zero, and this is a clear indication that the intensity values are equal or very close to each other, and as they are opposite, the result is zero because one cancels the other.

3-The molecule takes on the Chair position,and all readings are within the I.R. region.

4-Through the energy gap it becomes clear that the molecule is a semiconductor.

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