# DFT Study on the Three member Ring molecules (Thiirene , Seleniriene, tellurirene, and Poloniriene)

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## Abstract

Density functional theory calculations have been performed to get the optimized geometries and vibrational spectra (3N-6=9 fundamental frequencies along with their assignments and the corresponding IR absorption intensities) for the four three-member ring molecules (Thiirene , Seleniriene, tellurirene, and Poloniriene).It was shown that each one of the molecules belongs to Cs symmetry point group. The poloniriene has the higher values for C-X bond length, ∠CCX bond angle, entropy, and the lower values for the ∠CXC bond angle, dipole moment , reactivity , ring strain energy. Further more, some data on the bond dissociation energies, thermodynamics functions , UV/Visible transitions and the ring strain energy were also, reported.

## الخلاصة

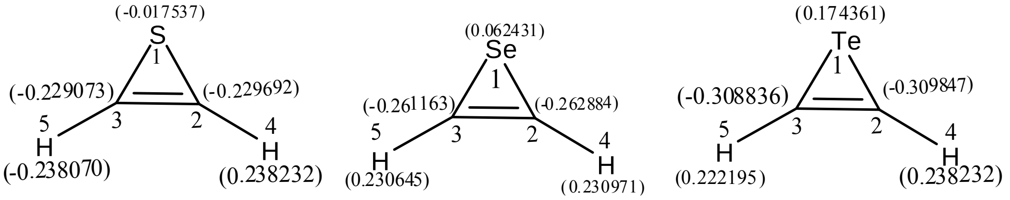
استعملت طريقة DFT ضمن برنامج Gaussian 03 لحساب الشكل الهندسي الأقل طاقة وكذلك للطيف الأهتزازي (3N-6=9 من ترددات الأنماط الاهتزازية الأساسية وشدة امتصاص الأشعة تحت الحمراء المقابلة لكل نمط و تشخيص الأنماط) لأربعة من الجزيئات ثلاثية الحلقة (الثايرين , سيلينيرين , تريلينيرين, و بولينيورين). تبين إن كل جريئة من هذه الجزيئات تعود آلي مجموعة التماثل $C_s$ . وجد ان لجزيئة بولينيورين القيمة الأكبر لطول الأصرة C-X, للزاوية ∠CCX , للأنتروبي والقيمة ألأصغر للزاوية ∠CXC, للفعالية , للعزم ثنائي القطب ولطاقة شد الحلقة مقارنة بباقي الجزيئات . تم تدوين طاقات تفكك الآصرة وبعض المعطيات عن الدوال الثرموداينمكية و ألانتقالات في منطقة الأشعة فوق البنفسجية والمرئية و طاقة شد الحلقة.

Keys words:-DFT calculation ,thiirene, seleniriene, tellurirene , and poloniriene.

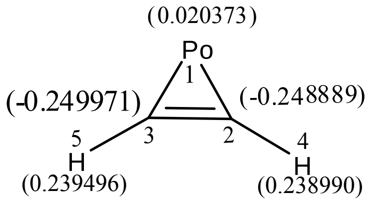
## Introduction

The chemistry of small ring molecules has been much scientific attention from both the experimental and the theoretical point of view .In particular three-membered ring hetrocycles have been investigated during the past 50 years (1) because some of them are typical "antiaromatic" system(2) and have been proposed as intermediates in a variety of reactions, for instance the thiirene is the primary adduct in the S($^1$D) + acetylene reaction(3). The selenirene is found as intermediate in the photolysis of 1,2,3-selenadizole(4) . The synthesis of thiirene and selenirene derivatives carrying bulky substituents was also reported(5).

In this work four three-member ring molecules; thiirene, seleniriene ,tellurirene, and Poloniriene, Fig.1, were investigated theoretically using the Density Functional Theory (DFT) method(6). However, except of thiirene, no any experimental and or theoretical studies concerning the molecular structures and the vibration spectra of these molecules were reported. .The calculation method was used to evaluate the equilibrium molecular structure, vibration spectrum , bond dissociation energies, thermodynamics functions , UV/Visible transitions and the ring strain energy of the four three-member ring molecules ; thiirene, seleniriene ,tellurirene, and Poloniriene.



a Thiirene b Seleniriene c Tellurirene



d Poloniriene

**Fig.1 Molecular structures of the four three-member ring molecules: a-thiirene ,b- Seleniriene, c-tellurirene, and d-Poloniriene along with Muilliken atomic charges in parenthesis's .**

## Computational Details

The vibrational wavenumbers were calculated using the Gaussian03 software package on a personal computer(6). The density functional theoretical (DFT) computations were performed at the B3LYP/SDDAll level of theory to get the optimized geometry (Fig. 1 and 2) and vibrational wave numbers of the normal modes of the title molecules, Tables 2,3,4,5,6. The DFT partitions the electronic energy $E=E_T+E_V+E_J+E_{XC}$, where $E_T$, $E_V$ and $E_J$ are electronic kinetic energy, electron nuclear attraction and electron–electron repulsion terms, respectively. The electron correlation is taken into account in the DFT via the exchange-correlation term $E_{XC}$, which includes exchange energy arising from the antisymmetry of quantum mechanical wavefunction and dynamic correlation in the motion of individual electrons, and it makes DFT dominant over the conventional Hartree–Fock (HF) procedure (7). DFT calculations were carried out with Becke's three-parameter hybrid model using the Lee–Yang–Parr correlation functional (B3LYP) method. Molecular geometries were fully optimized by Berny's optimization algorithm using redundant internal coordinates. All optimized structures were confirmed to be minimum energy conformations. Harmonic vibrational wavenumbers were calculated using analytic second derivatives to confirm the convergence to minima in the potential surface. At the optimized structure of the examined species, no imaginary wavenumber modes were obtained , proving that a true minimum on the potential surface was found. The optimum geometry was determined by minimizing the energy with respect to all geometrical parameters without imposing molecular symmetry constraints. The assignments of the calculated wavenumbers are aided by the animation option of MOLEKEL program, which gives a visual presentation of the vibrational modes (8, 9).

## Results and Discussion

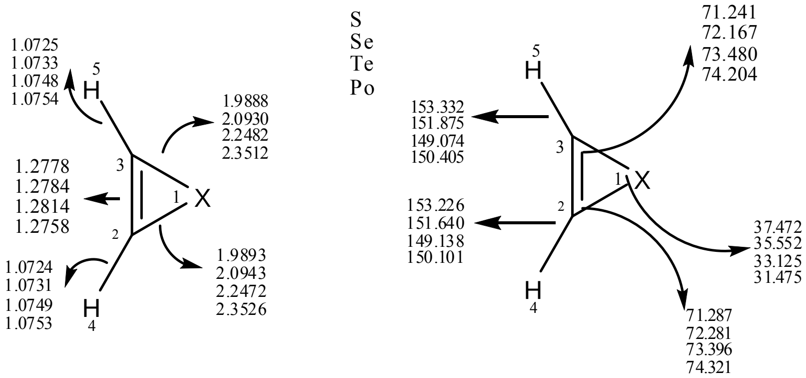


**Fig.2: Geometric parameters of the three-member ring molecule. X = S, Se , Te, and Po atoms respectively. Bond length in A$^{o}$ and bond angles in degrees.**

### 1-Geometry:

The geometrical parameters bond lengths and bond angles of each one of the four molecules were shown in Fig.2. The C-X bond length increases in the order thiireneI<seleniriene < tellurirene< poloniriene . The C=C bond length increases in the same order with the exception of poloniriene molecule. However , the contraction of the bond length in final molecule may be due to the present of the filled 4f orbital .The opposite sequence was shown for the CXC angles ; The thiirene molecule has the greater one , 37.472, due to the high electro negativity of S atom, while smallest one, 31.475 is for polonirene molecule , Fig.2. In addition to, the latter molecule has the lower dipole moment and is the less reactive one and has lower tendency to be reduced due to its lightest LUMO energy, Table 1 . Fig.1 shows the structure of each molecule along with the values of the Muilliken atomic charges in parenthesis. The charge cited on the X atom varies from negative value for S to positive ones for Se, Te and Po atoms. This may be due to the high electro negativity of first element, S, compared to that for Se, Te, and Po.

## 2-Vibration Spectra:

DFT calculation shows that all the four molecules are planar with the $C_s$ point group. From the character table, the 3N-6=9 normal vibration modes, of each one of these molecules, are distributed among the following irreducible representations, $\Gamma_9 = 7A^{-} + 2A^{=}$, where the $7A^{-}$ modes are in plane and the others are out of plane. In addition to, all the nine modes are IR and Raman active simultaneously.

The nine fundamental vibration frequencies, $cm^{-1}$, for each one of the four studied molecules along with their assignments and the corresponding IR intensities, $km.mol^{-1}$, were listed, Table 2. Some of physical properties; force constant, $mdyne.cm^{-1}$ , reduced mass, $Kg^{-1}$, Raman activity, depolarization ratio of each one of the nine fundamental vibration modes and for each one of the studied molecules were also shown, Tables 3,4,5,6.

From Table 2, it is obvious that the highest frequency values are the CH stretch modes, which are localized along the C-H bonds. The $v_1$ mode, , has larger frequency value than the other one, $v_2$ .The next higher one is $v_3$ , the C=C stretch , mode. The C-H and C=C bonds have, also, the higher force constants, and the latter is the highest one due to presence of the double bond, Tables 3,4,5,6. In addition to, the stretch vibration modes have the highest Raman scattering activity. The values of depolarization ratio for the unpolarized incident light are higher than that for plane incident light. The value of 0.75 for the depolarization ratio, for some vibration modes, indicates that these modes are depolarized bands and the modes with depolarization ratio less than 0.75 are the polarized bands, Tables 3,4,5,6.

## 3-Bond dissociation energy

The bond dissociation energy, D, in $Kcal.mol^{-1}$, of the C=C bond was calculated using the following equation [(10)],

$$\nu = 143.3(D - c_1)^{1/2}$$

where $\nu$, in $cm^{-1}$, is the uncoupled stretching frequency, $c_1$ is constant characteristic of the two bonded atoms. The $c_1$ value for Carbon- carbon bond , 39.7, is used to calculate the D for the C=C bonds , Table 7. It was shown that the highest D, value is that for thiirene molecule due to its smallest C=C bond length, Table 1, and in turn the highest bond order .On the other hand , the tellurirene has the lower D value due to its long C=C bond length . However, compared with tellurirene , the increment in dissociation energy of poloniriene may be due to the shortage of C=C bond length and in turn increases the bond order of the bond. This may be due to the presence of the occupation 4f orbital in Po atom.

## 4-Thermodynamics functions:

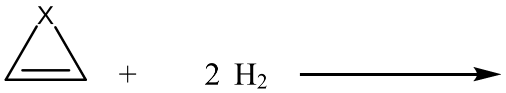
Thermodynamics functions for the studied molecules were listed in Table.7. It was shown that the highest value of entropy, $S^o$, is for poloniriene molecule and the lowest one is for thiirene. In the former molecule, the Po atom has a small inductive effect compared with that of S atom .So, the lone pair electrons, in poloniriene, are less bounded and consequently have the more freely motion. Therefore, the poloniriene has the higher $S^o$, Table.7.The reverse sequence is shown for $G^o$ and the poloniriene has the lowest value, -0.200 $Kcal.mol^{-1}$, Table 7.

## 5-Theoretical UV/ Visible transitions

Theoretical UV/ Visible transitions for thiirene , seleniriene, tellurirene, and poloniriene molecules were shown in Tables 8, 9, 10, 11 respectively. From these Tables, it is shown that the first excited state , corresponding to the HOMO-LUMO energy transition for the molecule , has the lower energy (the longer wave length) than the second and third transitions. This may be attributed to the small energy gap of the HOMO-LUMO transition compared with that of the other two transitions. Also, these transitions may be assigned as $n \rightarrow \Pi^*$, $n \rightarrow \sigma^*$ and $\Pi \rightarrow \Pi^*$.In addition to, the energy of HOMO-LUMO transition are increased as the following order: thiirene >seleniriene>tellurirene>poloniriene. The high HOMO-LUMO transition energy for the thiirene may be attributed to the higher electro negativity of S atom compared with that of Se, Te, and Po atoms . This consequently leads to restrict the motion of the electrons and in turn a more energy is required for transition. This sequence is valid also for the second and third excited states series and for the four molecules with exception of poloniriene, Table 12. The anomalous of the last molecule may be, as we mentioned before, due to the present of the filled 4f orbital of the Po atom.

## 6-Ring strain

Ring strain is the tendency of a cyclic molecule to destabilize when its atoms are in non-favorable high-energy spatial orientations. It consists primarily of two different kinds of strain, the torsion and angle strains. The hydrogenation energy (11) can be used as a measure of ring strain in the three member ring molecules by calculating $\Delta H$ for the following reaction,



$CH_3CH_2X$ H , X= S , Se , Te , Po

where the energy strain is equal to the negative $\Delta H$.,

The values of energy ring strain of the studied molecules have been shown in Table 13. It is obvious to show that energy strain increases as the electro negativity of the X atom increased .So, the highest strain is for thiirene and the least one is for poloniriene.

**Table.1: Some physical properties of the four three-member ring molecules involved in this study by atomic units, a.u .**

| | (Thiirene) | (Seleniriene) | (Tellurirene) | Poloniriene |
|---|---|---|---|---|
| $E_{HOMO}$, A.U | -0.21093 | -0.20300 | -0.19551 | -0.18729 |
| $E_{LUMO}$, A.U | -0.02770 | -0.03863 | -0.05752 | -0.05528 |
| $\Delta$ $E_{HOMO-LUMO}$, A.U | -0.18323 | -0.16437 | -0.13799 | -0.13201 |
| E(RB+HF-LYP], A.U | -22.5914 | -21.7681 | -20.5043 | -20.3485 |
| Dipole moment, Debye | 2.7785 | 2.2863 | 1.8324 | 1.4862 |

**Table.2: Correlations of frequencies in cm$^{-1}$ along with their corresponding IR intensity , for two decimal only , in km.mol$^{-1}$(in parenthesis's) and their assignments for the studied four molecules.**

| | Thiirene | Seleniriene | telluriene | poloniriene | Assignment* |
|---|---|---|---|---|---|
| $V_1$ | 3413(8.02) | 3402(7,75) | 3378(7.94) | 3372(7.82) | CH s st. |
| $V_2$ | 3349(25.84) | 3340(20.91) | 3321(14.73) | 3311(19.02) | CH as.st |
| $V_3$ | 1761(17.09) | 1750(28.24) | 1730(53.31) | 1736(68.82) | C=C st |
| $V_4$ | 905(56.75) | 890(73.62) | 886((89.10) | 851(101.52) | $\delta$ CH |
| $V_5$ | 883(0.12) | 860(3.54) | 842(15.66) | 794(33.25) | $\delta$ CH |
| $V_6$ | 567(11.94) | 460(9.87) | 412(10.44) | 383(0.85) | Ring elongation($\delta$ Po CC) |
| $V_7$ | 360(0.25) | 368(0.57) | 389(1.31) | 366(9.63) | $\delta$ XCC(Ring elongation) |
| $V_8$ | 754(0.00) | 756(0.01) | 761(0.00) | 739(0.00) | $\gamma$ CH |
| $V_9$ | 661(165.47) | 660(170.54) | 657(174.75) | 638(141.98) | $\gamma$ CH |

*assignments in the parenthesis's, column 6, are for the polonirene molecule. and X refers to S, Se and Te atoms ; s: symmetric, st: stretching, $\delta$ : in plane bending, s: symmetric, as: antsymmetric, $\gamma$ : out of plane bending.

**Table.3: Some physical properties of vibration spectrum of thiirene molecule$^{*}$..**

| | Force constant | Reduced mass | IR intensity | Raman Activity | Depolar (p) | Depolar (u) | assignments |
|---|---|---|---|---|---|---|---|
| $V_1$ | 7.9581 | 1.1598 | 8.0248 | 118.6267 | 0.1210 | 0.2158 | CH s st. |
| $V_2$ | 7.1569 | 1.0833 | 25.8397 | 88.1499 | 0.7500 | 0.8571 | CH as.st |
| $V_3$ | 9.0881 | 4.9753 | 17.0867 | 55.5927 | 0.1093 | 0.1971 | C=C st |
| $V_4$ | 0.5914 | 1.2240 | 56.7542 | 0.5249 | 0.7493 | 0.8567 | $\delta$ CH |
| $V_5$ | 0.4795 | 1.0443 | 0.1241 | 0.5769 | 0.1655 | 0.2840 | $\delta$ CH |
| $V_6$ | 2.5158 | 13.2720 | 11.9436 | 24.1307 | 0.3691 | 0.5391 | Ring elongation |
| $V_7$ | 0.4725 | 6.1786 | 0.2499 | 20.6486 | 0.7500 | 0.8571 | $\delta$ SCC |
| $V_8$ | 0.4926 | 1.4717 | 0.0001 | 1.6302 | 0.7500 | 0.8571 | $\gamma$ CH |
| $V_9$ | 0.2921 | 1.1328 | 165.4654 | 0.6154 | 0.7500 | 0.8571 | $\gamma$ CH |

*Force constant, mdyne /A$^{o}$ ; Reduced mass, amu; IR intensity, km.mol$^{-1}$; Raman activity , A**4/amu; for symbols and abbreviations, see Table 2

**Table.4 Some physical properties of vibration spectrum of seleniriene molecule*.**

| | Force constant | Reduced mass | IR intensity | Raman Activity | Depolar (p) | Depolar (u) | Assignment |
|---|---|---|---|---|---|---|---|
| $V_1$ | 7.8894 | 1.1572 | 7.7517 | 139.9744 | 0.1182 | 0.2114 | CH s st. |
| $V_2$ | 7.1196 | 1.0833 | 20.9119 | 113.9839 | 0.7495 | 0.8568 | CH as.st |
| $V_3$ | 9.0927 | 5.0377 | 28.2404 | 61.4217 | 0.0969 | 0.1767 | C=C st |
| $V_4$ | 0.5706 | 1.2230 | 37.6295 | 0.2169 | 0.7241 | 0.8400 | $\delta$ CH |
| $V_5$ | 0.4515 | 1.0364 | 3.5401 | 1.4730 | 0.0868 | 0.1597 | $\delta$ CH |
| $V_6$ | 1.4064 | 11.2877 | 9.8686 | 18.4862 | 0.3959 | 0.5672 | Ring elongation |
| $V_7$ | 0.4355 | 5.4517 | 0.5665 | 19.0829 | 0.7499 | 0.8571 | $\delta$ SCC |
| $V_8$ | 0.4929 | 1.4645 | 0.0133 | 1.1282 | 0.7500 | 0.8571 | $\gamma$ CH |
| $V_9$ | 0.2902 | 1.1302 | 170.5440 | 0.7714 | 0.7500 | 0.8571 | $\gamma$ CH |

* For symbols and abbreviations, see Tables 2 and 3

**Table.5: Some physical properties of vibration spectrum of tellurirene molecule*.**

| | Force constant | Reduced mass | IR intensity | Raman Activity | Depolar (p) | Depolar (u) | Assignment |
|---|---|---|---|---|---|---|---|
| $v_1$ | 7.7472 | 1.1519 | 7.9393 | 192.5488 | 0.1242 | 0.2209 | CH s st. |
| $v_2$ | 7.0831 | 1.0831 | 14.7318 | 160.1534 | 0.7500 | 0.8571 | CH as.st |
| $v_3$ | 9.1271 | 5.1759 | 53.3115 | 70.6951 | 0.0920 | 0.1685 | C=C st |
| $v_4$ | 0.5705 | 1.2329 | 89.1078 | 0.1531 | 0.7420 | 0.8519 | $\delta$ CH |
| $v_5$ | 0.4293 | 1.0282 | 15.6584 | 4.0686 | 0.0495 | 0.0944 | $\delta$ CH |
| $v_6$ | 1.0747 | 10.7592 | 10.4458 | 19.3916 | 0.4642 | 0.6340 | Ring elongation |
| $v_7$ | 0.4470 | 5.0220 | 1.3120 | 19.9006 | 0.7497 | 0.8570 | $\delta$ SCC |
| $v_8$ | 0.4953 | 1.4507 | 0.0013 | 0.5544 | 0.7500 | 0.8571 | $\gamma$ CH |
| $v_9$ | 0.2872 | 1.1298 | 174.7508 | 0.6753 | 0.7500 | 0.8571 | $\gamma$ CH |

* For symbols and abbreviations, see Tables 2 and 3 .

**Table.6 :Some physical properties of vibration spectrum of Poloniriene molecule*.**

| | Force constant | Reduced mass | IR intensity | Raman Activity | Depolar (p) | Depolar (u) | Assignment |
|---|---|---|---|---|---|---|---|
| $v_1$ | 7.7442 | 1.1562 | 7..8255 | 299.0011 | 0.1292 | 0.2288 | CH s st. |
| $v_2$ | 6.9943 | 1.0829 | 19.0249 | 187.2077 | 0.7497 | 0.8569 | CH as.st |
| $v_3$ | 8.8553 | 4.9882 | 68.8160 | 70.2930 | 0.0921 | 0.1687 | C=C st |
| $v_4$ | 0.5279 | 1.2359 | 101.5181 | 0.8159 | 0.7407 | 0.8510 | $\delta$ CH |
| $v_5$ | 0.3805 | 1.0249 | 33.2551 | 11.2477 | 0.2678 | 0.4225 | $\delta$ CH |
| $v_6$ | *0.4164* | 4.8076 | 0.8482 | 19..1339 | 0.7493 | 0.8567 | $\delta$ SCC |
| $v_7$ | 0.8420 | 10.6746 | 9.6301 | 16.1567 | 0.2755 | 0.4320 | Ring elongation |
| $v_8$ | 0.4694 | 1.4591 | 0.0020 | 0.5130 | 0.7500 | 0.8571 | $\gamma$ CH |
| $v_9$ | 0.2698 | 1.1255 | 141.9838 | 1.9935 | 0.7500 | 0.8571 | $\gamma$ CH |

* For symbols and abbreviations, see Tables 2 and 3

**Table.7: Thermodynamics functions and bond dissociation energies for the thiirene, seleniriene, tellurirene , and poloniriene molecules***

| Molecule | $U^o$ | $H^o$ | $S^o$ | $G^o$ | $A^o$ | D | Energy Strain, |
|---|---|---|---|---|---|---|---|
| Thiirene | 20.408 | 21.000 | 63.050 | 2.202 | 1.610 | 190.717 | 106.732 |
| Seleniriene | 20.216 | 20.808 | 65.853 | 1.174 | 0.582 | 188.836 | 99.581 |
| Tellurirene | 20.076 | 20.668 | 67.554 | 0.527 | -0.065 | 185.447 | 93.559 |
| Poloniriene | 19.866 | 20.458 | 69.378 | -0.200 | -0.819 | 186.459 | 88.322 |

* $U^o$ ; $H^o$; $G^o$; $A^o$ ;D ; and energy strain, $Kcal.mol^{-1}$ ; $S^o$ , $cal.mol^{-1}.K^{-1}$

**Table 8:Theoretical UV/ Visible transitions of thiirene molecule.**

| | First Excited State | Second Excited State | Third Excited State |
|---|---|---|---|
| Excitation energy, nm | 339.23 | 335.25 | 307.72 |
| Oscillator Strength | 0.0000 | 0.0002 | 0.0024 |
| Occupied MO | 8 | 8 | 8 |
| Unoccupied MO | 10 | 9 | 11 |
| Coefficient | 0.68442 | 0.66341 | 0.67973 |

**Table 9:Theoretical UV/ Visible transitions of Selenirene molecule**

| | First Excited State | Second Excited State | Third Excited State |
|---|---|---|---|
| Excitation energy, nm | 387.21 | 370.53 | 313.17 |
| Oscillator Strength | 0.0000 | 0.0001 | 0.0011 |
| Occupied MO | 8 | 8 | 8 |
| Unoccupied MO | 9 | 10 | 11 |
| Coefficient | 0.68491 | 0.66351 | 0.68273 |

**Table 10:Theoretical UV/ Visible transitions of Tellurirene molecule**

| | First Excited State | Second Excited State | Third Excited State |
|---|---|---|---|
| Excitation energy, nm | 472.85 | 395.31 | 320.47 |
| Oscillator Strength | 0.0000 | 0.0003 | 0.0004 |
| Occupied MO | 8 | 8 | 7, 8* |
| Unoccupied MO | 9 | 10 | 10, 11 |
| Coefficient | 0.68108 | 0.66139 | 0.10548, 0.68544* |

* $8 \rightarrow 11$ transition

**Table 11:Theoretical UV/ Visible transitions of Poloniriene molecule**

| | First Excited State | Second Excited State | Third Excited State |
|---|---|---|---|
| Excitation energy, nm | 494.69 | 470.96 | 328.48 |
| Oscillator Strength | 0.0000 | 0.0007 | 0.0001 |
| Occupied MO | 8 | 8 | 7, 8* |
| Unoccupied MO | 9 | 10 | 10, 11 |
| Coefficient | 0.68433 | 0.66332 | -0.21885, 0.66401* |

* $8 \rightarrow 11$ transition

**Table 12: comparison of theoretical UV/ Visible transitions energies of the studied molecule***

| Molecule | First Excited State, nm | Second Excited State, nm | Third Excited State, nm |
|---|---|---|---|
| Thiirene | 339.23 | 335.25 | 307.72 |
| seleniriene | 387.21 | 370.53 | 313.17 |
| tellurirene | 472.85 | 395.31 | 320.47 |
| Polloniriene | 494.69 | 470.96 | 328.48 |

*See Tables 8, 9, 10, 11.

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