Studying of Frequencies, Normal Modes of Vibration and Electronic Charge Densities of 5Radialene molecule

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Abstract

PM3 and DFT (6-311G/ B3LYP) level calculations were carried out for the 5Radialene molecule, which is exhibit D_{5h} symmetry. The obtained equilibrium geometry was applied for the calculation of all 3N−6 vibration frequencies, and for the analysis of its normal coordinates and symmetry species, in addition to some physical properties such as heat of formation, total energy, dipole moment and energy difference of HOMO and LUMO levels ($\Delta E_{LUMO-HOMO}$), using Gaussian-03 program. The so calculated frequencies according to DFT (6-311G/ B3LYP) fall in the ranges;

νCH_2 str. (3016-3098 cm^{-1}), νC=C str. (1662-1709cm^{-1}), νring (C-C str.) (1268-1464 cm^{-1}). δCH_2 (890-1317cm^{-1}), (δCCC) (562-631cm^{-1}), γCH_2 (738-946cm^{-1}) and γring (γCCC) (14-805cm^{-1}), and according to PM3 fall in the ranges;

νCH_2 str. (3124-3138cm^{-1}), νC=C str. (1873-1939cm^{-1}), νring str. (C-C str.) (1289-1430cm^{-1}). δCH_2 (946-1503cm^{-1}), (δCCC) (549-777cm^{-1}), γCH_2 (673-1007cm^{-1}) and γring (γCCC) (54-785cm^{-1}).

Other interesting correlations were also be obtained for the frequencies of similar vibrations. Distribution of electronic charge density on atoms of 5Radialene molecule were also calculated and studied.

Keywords: 5Radialene, Frequency, Electronic Charge Density.

دراسة ترددات الاهتزاز و الاحداثيات الداخلية و كثافة الشحنة الالكترونية لجزيئة 5 راديالين

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الخلاصة

تضمن البحث استخدام إحدى طرق ميكانيك الكم التقريبية شبه التجريبية Semi-empirical method (parameter model 3 (PM3) و طريقة DFT (6-311G/ B3LYP) الأساسية غير التقريبية باستخدام برنامج Gaussian-03 في حساب و تصنيف ترددات اهتزاز طيف الأشعة تحت الحمراء لجزيئه 5Radialene و بعدد 3N-6 وتشخيصها تكافؤيا و تماثليا، مع بعض الصفات الفيزياوية كحرارة التكوين و الطاقة الكلية وعزم ثنائي القطب و الفرق الطاقي $\Delta E_{HOMO-LUMO}$ -- الخ، عند الشكل الهندسي التوازني. تم الحصول على القيم الآتية لترددات الاهتزاز وفق نظرية دوال الكثافة DFT :

νCH_2 str. (3016-3098 cm^{-1}), νC=C str. (1662-1709cm^{-1}), ring (C-C str.) (1268-1464 cm^{-1}). δCH_2 (890-1317cm^{-1}), (δCCC) (562-631cm^{-1}), γCH_2 (738-946cm^{-1}) and γring (γCCC) (14-805cm^{-1}).

و على القيم الآتية وفق طرقة الحساب التقريبية PM3 :

νCH_2 str. (3124-3138cm^{-1}), νC=C str. (1873-1939cm^{-1}), νring (C-C str.) (1289-1430cm^{-1}). δCH_2 (946-1503cm^{-1}), (δCCC) (549-777cm^{-1}), γCH_2 (673-1007cm^{-1}) and γring (γCCC) (54-785cm^{-1}).

كما تم حساب و دراسة توزيع الكثافة الالكترونية على ذرات هذه الجريئة.

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1. Introduction

Radialenes are alicyclic compounds in which all ring atoms are sp2-hybridized and carry exocyclic double bonds. They are a class of compounds exhibiting very interesting structural and electronic properties. The cooperative involvement of the latter has also been considered [1-5] in organic conducting, or ferromagnetic, solid-state. Two main approaches for the synthesis of these compounds have been studied: (i) the olefin-forming reactions at an already existing cycloalkane ring; (ii) the metal-induced cyclo-oligomerization reactions of suitable [n] cumulenes. While a number of 3, 4, and 6Radialenes have been obtained [6-8]. Florence Geneste et. al. studied the experimental as well as the theoretical results by ab initio calculations of many molecules which 5Radialene is the central ring of these molecules [9]. The preparations of 5Radialenes proved to be far more difficult. 5Radialene can be stabilized by incorporating the exocyclic double bonds into a cyclic such as the conformation of bucybowl corannullene [10-14] which is the fragment of bulckybowl fullerene (C_{60}) [15]. 5Radialene is the conformation of the central ring of corannullene and bulckybowl fullerene (C_{60}) as shown in Figure 1, which has been synthesized but the preparations of 5Radialene is still difficult, and no experimental vibration frequencies are known.

In the present work, we applied the PM3 method [16] and the B3LYP-Density Functional Theory (DFT) [17]; They are known to yield good vibration frequency values for the 5Radialene, and evaluated all (3N-6) vibration frequencies of 5Radialene and assigned them to the corresponding normal coordinates. IR absorption intensities were calculated applying the DFT method and the 6-311G gaussian basis set. For the analysis of the normal coordinates the Graphical pictures of gaussian program was used [18].

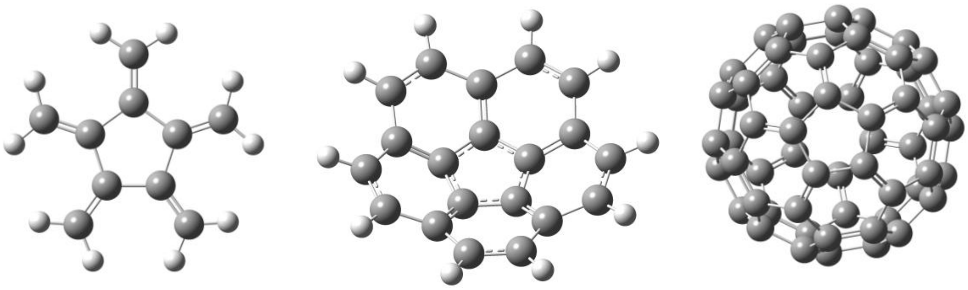

(a) **(b)** **(c)**

Figure 1- Equilibrium geometries of (a) 5Radialene, (b) Coranulene, and (c) Fullerene molecules.

2. Results and Discussion

5Radialene is a planer molecule with D_{5h} point group, Table 1 shows the calculated geometric parameters (bond lengths and bond angles) according to its symmetry, and the table also included some physical and energetic properties. Figure 2 shows the numbering of the atoms for 5Radialene molecule calculated at its equilibrium geometry (minimize energy).

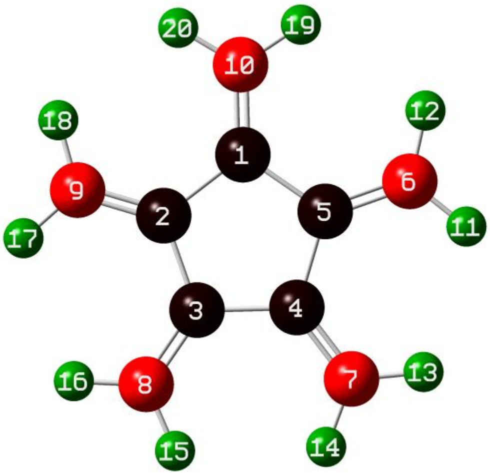


Figure 2- Numbering of the atoms of 5Radialene molecule.

Table 1- PM3 and DFT (6-311G/ B3LYP) calculated geometric structures of 5Radialene molecule.

Description of bond lengths & angles	**Bond lengths (Å) & angles (deg)**	
	PM3	**DFT (6-311G/ B3LYP)**
C1-C2	**1.4751**	**1.4930**
C1-C5	**1.4751**	**1.4930**
C1-C10	**1.3336**	**1.3416**
C10-H19	**1.0867**	**1.0813**
< C2C1C5	**108.000**	**107.999**
< C2C1C10	**126.000**	**126.000**
< C1C10H19	**122.570**	**121.995**
< H19C10H20	**114.726**	**116.009**
Molecular formula	$C_{10}H_{10}$	
m.wt. (g/mol.)	**130.189**	
Point group	D_{5h}	
ΔH_f **(kcal/mol)** ΔH_f **(kJ/ mol)**	**80.875** **338.381**	**80.875** **386.984**
Electronic energy (eV)	**-6962.544**	**--------**
Core-core repulsion (eV)	**5626.320**	**--------**
Ionization potential (eV)	**9.112**	**--------**
E_{LUMO} **(eV)**	**-0.395**	**-0.381**
E_{HOMO} **(eV)**	**-9.113**	**-9.088**
$\Delta E_{LUMO-HOMO}$ **(eV)**	**8.718**	**8.708**
Dipole moment (Debye)	**0.002**	**0.000**

3. Vibration frequencies of 5Radialene.

5Radialene molecule posses 54 fundamental vibrations. Inspection of its irreducible representations, as defined by the symmetry character table, results in the following modes of vibration;

Γvibration= Γtotal- (Γrotationn+ Γtranslation)= 3N–6= 60– 6= 54= $4A_1' + 3A_2' + 7E_1' + 8E_2' + 1A_1'' + 2A_2'' + 3E_1'' + 4E_2''$

These are 54 modes of vibration, 23 of which are Raman active ($4A_1'$ (polarized) + $8E_2'$ (depolarized) + $3E_1''$ (depolarized), and 16 IR active ($7E_1' + 2A_2''$). The rest are both IR and Raman inactive.

Relative to the бh reflection the vibration modes are classified as:

a- symmetric modes with respect to бh (+бh).

$\Gamma_{In\text{-}plane} = 2N-3 = 37 = 4A_1' + 3A_2' + 7E_1' + 8E_2'$

b- antisymmetric modes with respect to бh (-бh).

$\Gamma_{Out\ of\ plane} = N-3 = 17 = 1A_1'' + 2A_2'' + 3E_1'' + 4E_2''$

It was possible to assign all the vibration modes both symmetrically and according to their valence nature. The valence assignment could be done considering the calculated graphical pictures of all vibration modes as obtained applying the Gaussian 03 program Figure 2.

Table 2 shows the calculated vibration frequencies and IR absorption intensities of the 5Radialene molecule results applying the PM3 and DFT methods. Commonly known, the vibrations with (intensity= 0.0) are IR forbidden, those with (intensity≠ 0.0) are IR allowed. The vibration modes in Table 2 are classified according to the Herzberg scheme [19]. Figure 3 shows the graphycal pictures for some modes of vibration of the 5Radialene molecule, as calculated applying the DFT method. No experimental vibrational frequencies data for this molecule are available in the literature to compare them with our calculated results. Also the complete normal coordinate analysis on the symmetry and the valence basis of all its 3N−6 vibration modes of this molecule is still missing.

Table 2- Vibrational frequencies and IR absorption intensities for 5Radialene molecule.

DFT (6-311G/ B3LYP)		**PM3**	**Symmetry and Description**	
Intensity km/mol	**Freq. cm^{-1}**	**Freq. cm^{-1}**		
In plane modes of vibration				
				A$_1$'
0.0000	**3022**	**3124**	**CH$_2$ asy str.**	ν_1
0.0000	**1685**	**1939**	**C=C str. + δCH$_2$ (scissoring)**	ν_2
0.0000	**1503**	**1317**	**δCH$_2$ (scissoring)**	ν_3
0.0000	**631**	**777**	**δRing (δCCC str.) (breathing)**	ν_4
				A$_2$'
0.0000	**3091**	**3138**	**CH$_2$ asy. str.**	ν_5
0.0000	**1166**	**1056**	**δCH$_2$ (rocking) + δring (clock-anti clock)**	ν_6
0.0000	**584**	**580**	**δring (clock-anti clock) + δCH$_2$ (rocking)**	ν_7
				E$_1$'
28.571	**3095**	**3137**	**CH$_2$ asy str.**	ν_8
28.571	**3095**	**3137**	**CH$_2$ asy. str.**	ν_9
19.348	**3019**	**3125**	**CH$_2$ sym. str.**	ν_{10}
19.348	**3019**	**3125**	**CH$_2$ sym. str.**	ν_{11}
9.1517	**1662**	**1873**	**C=C str. + δCH$_2$ (scissoring)**	ν_{12}
9.1517	**1662**	**1873**	**C=C str. + δCH$_2$ (scissoring)**	ν_{13}
46.590	**1486**	**1340**	**δCH$_2$ (scissoring) + δring**	ν_{14}
46.590	**1486**	**1340**	**δCH$_2$ (scissoring) + δring**	ν_{15}
20.533	**1216**	**1196**	**δCH$_2$ (rocking) + δring**	ν_{16}
20.533	**1216**	**1196**	**δCH$_2$ (rocking) + δring**	ν_{17}
3.1181	**843**	**868**	**δring + δCH$_2$ (rocking)**	ν_{18}
3.1181	**843**	**868**	**δring + δCH$_2$ (rocking)**	ν_{19}
1.6484	**341**	**305**	**δC=C + δCH$_2$ (rocking)**	ν_{20}
1.6484	**341**	**305**	**δC=C + δCH$_2$ (rocking)**	ν_{21}
				E$_2$'
0.0000	**3098**	**3135**	**CH$_2$ asy str.**	ν_{22}
0.0000	**3098**	**3135**	**CH$_2$ asy. str.**	ν_{23}
0.0000	**3016**	**3128**	**CH$_2$ asy str.**	ν_{24}
0.0000	**3016**	**3128**	**CH$_2$ asy. str.**	ν_{25}
0.0000	**1709**	**1887**	**C=C str. + (CCC str.) ring puck. + δCH$_2$ (scissoring)**	ν_{26}
0.0000	**1709**	**1887**	**C=C str. + (CCC str.) ring puck. + δCH$_2$ (scissoring)**	ν_{27}
0.0000	**1464**	**1430**	**C-C str. + δCH$_2$ (rocking)**	ν_{28}
0.0000	**1464**	**1430**	**C-C str. + δCH$_2$ (rocking)**	ν_{29}
0.0000	**1268**	**1289**	**C-C str. + δCH$_2$ (rocking)**	ν_{30}
0.0000	**1268**	**1289**	**C-C str. + δCH$_2$ (rocking)**	ν_{31}
0.0000	**946**	**890**	**δCH$_2$ (rocking) + δring**	ν_{32}
0.0000	**946**	**890**	**δCH$_2$ (rocking) + δring**	ν_{33}
0.0000	**562**	**549**	**δring (δCCC)**	ν_{34}
0.0000	**562**	**549**	**δring (δCCC)**	ν_{35}
0.0000	**360**	**289**	**δC=C + δCH$_2$ (rocking)**	ν_{36}
0.0000	**360**	**289**	**δC=C + δCH$_2$ (rocking)**	ν_{37}
Out of plane modes of vibration				
				A$_1$"
0.0000	**648**	**642**	**γCH$_2$ (twisting)**	ν_{38}
				A$_2$"
249.223	**946**	**1007**	**γCH$_2$ (wagging)**	ν_{39}

10.716	**241**	**229**	**γring + γCH_2 (wagging)**	**ν_{40}**
				E_1''
0.0000	**937**	**1009**	**γCH_2 (wagging)**	**ν_{41}**
0.0000	**937**	**1009**	**γCH_2 (wagging)**	**ν_{42}**
0.0000	**738**	**673**	**γCH_2 (twisting) + γring**	**ν_{43}**
0.0000	**738**	**673**	**γCH_2 (twisting) + γring**	**ν_{44}**
0.0000	**349**	**364**	**γring + γCH_2 (twisting)**	**ν_{45}**
0.0000	**349**	**364**	**γring + γCH_2 (twisting)**	**ν_{46}**
				E_2''
0.0000	**938**	**1022**	**γCH_2 (wagging)**	**ν_{47}**
0.0000	**938**	**1022**	**γCH_2 (wagging)**	**ν_{48}**
0.0000	**805**	**785**	**γring + γCH_2 (wagging)**	**ν_{49}**
0.0000	**805**	**785**	**γring + γCH_2 (wagging)**	**ν_{50}**
0.0000	**615**	**554**	**γring + γCH_2 (twisting)**	**ν_{51}**
0.0000	**615**	**554**	**γring + γCH_2 (twisting)**	**ν_{52}**
0.0000	**14**	**54**	**γring + γCH_2 (wagging)**	**ν_{53}**
0.0000	**14**	**54**	**γring + γCH_2 (wagging)**	**ν_{54}**

γ: out of plane bending vibration. , δ :in-plane bending vibration.
Scaling factors: 0.96 (CH str.) for all DFT (B3LYP/6-311G) frequencies, [20].

The valance assignments of the modes are as follows:

- νCH_2 stretching vibrations

The frequency values range from ((3016-3098 cm^{-1}), showing the following correlations:

ν_{asym} (=CH_2 str.) (3095 cm^{-1}) (E_1') > ν_{sym} (=CH_2 str.) (3022 cm^{-1}) (A_1')

The highest intensity is 28.571km/mole due to $\nu_{8,9}$ (3095 cm^{-1}) **(E_1')**.

- νRing (C=C) stretching vibrations.

The calculated C=C stretching vibration frequencies range from (1662-1709 cm^{-1}), showing the following correlation;

ν_{asym}. (C=C str.) (1709 cm^{-1}) (E_2') > ν_{sym}. (C=C str.) (1685 cm^{-1}) (A_1')

The highest intensity is 9.151km/mole due to $\nu_{12,13}$ (1662 cm^{-1}) **(E_1')**

- νRing (C-C) stretching vibrations

The C-C vibration modes, located at C atoms of pentane ring , as can be seen from the atomic displacement vectors. Their frequencies are lower than those of the C=C vibration modes. According to the calculated results, the range of these frequencies is (1268-1464 cm^{-1}).

- δCH_2 in-plane bending vibrations

The frequency values range from (946-1503 cm^{-1}), showing the following correlations:

ν_{sym} (δCH_2) (scissoring)(1503 cm^{-1})(A_1') > ν_{asym} (δCH_2) (rocking)(1166 cm^{-1})(A_2'),
and:
$\nu_{asym}\delta CH_2$ (scissoring)(1486 cm^{-1}) (E_1') > ν_{asym} δCH_2 (rocking))(1216 cm^{-1})(E_1')

The highest intensity is 46.590km/mole due to ν_{14} (1486 cm^{-1}) **(E_1')**

- δRing in-plane bending vibrations (δCCC)

The deformation (δCCC) vibrations are of smaller values. According to their assignment, they fall in the range (562-631 cm^{-1}). These models include the expected clock and breathing and puckering vibration motions with the following relations:

$\nu_{asym.}$ (δCCC) (843 cm^{-1}) (E_1') > $\nu_{sym.}$ (δCCC) (631cm^{-1}) (A_1')

The highest intensity is 3.118km/mole due to ν_{18} (843 cm^{-1}) **(E_1')**

- γCH_2 out of plane vibration

The calculated frequencies range is (738-946 cm^{-1}), with the following relations:

ν_{asym} γCH_2 (wagging)(938 cm^{-1}) (E_2'') > $\nu_{asym}\gamma CH_2$(twisting) (738 cm^{-1}) (E_1'')

The highest intensity is 249.223 km/mole due to ν_{39}(946 cm^{-1}) **(A_2'')**

- γRing out of plane vibrations (γCCC)

The ring out of plane vibrations (γCCC), show frequencies values range **(14-805 cm^{-1}).**

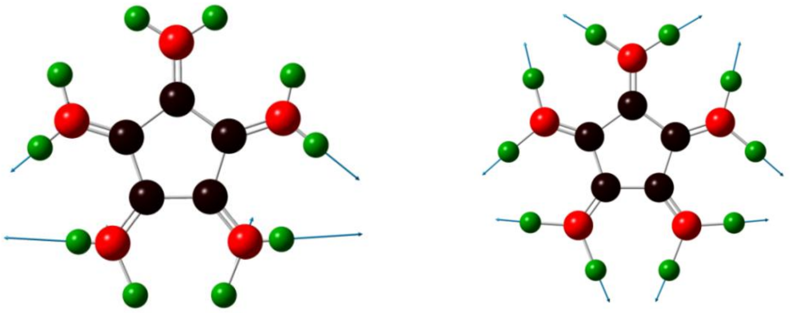
The highest intensity is 10.716 km/mole due to ν_{40}(241 cm^{-1}) **(A_2'')**

Finally, as it was studied previously [21], calculations of the charge densities show that they were mainly concentrated at the methylene carbon atoms (σ=C) for the negatively charges and at hydrogen atoms for the positively charges (σ-H). The carbon atoms have diminishing charges from outer to centre **(σ=C > σ—C).** The H atoms are positively charged, the C atoms are of the negative charge as in Figure 4. Distinguishing between the ring carbon atoms, C_{ring}, and the external methylene carbon atoms,

C_{ext}, it is found that the electronic charge densities at the pentane ring carbon atoms, -C_{ring}, are smaller than those at the external methylene carbon atoms, This seems to contradict the assumption of an sp hybridization at the ring atoms, which should possess higher electron affinities than expected. Two factors might explain these results:

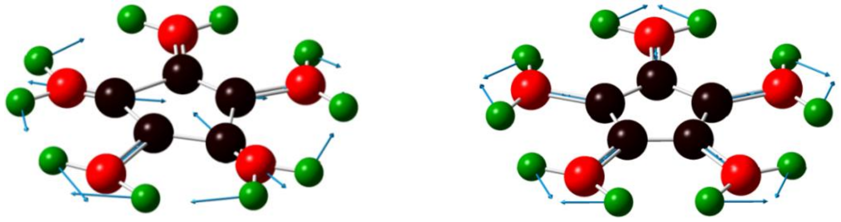
1. The delocalization of the ring electrons, causing a partial distribution of the electrons in the bond regions besides the localization at the C atoms, since a Mulliken population analysis was drawn to describe the electron distribution in the molecule.

2. For the external methylene carbon atoms a partial shift of electrons exists from the neighbored H atoms to C, as might be viewed considering the calculated electron densities at the H atoms, as shown in Figure 4.



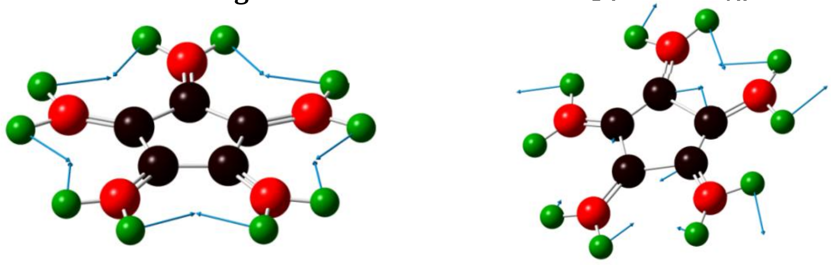
ν_{22}, **3098 cm^{-1}**
νCH_2 asymmetric stretching

ν_1, **3022 cm^{-1}**
νCH_2 symmetric stretching



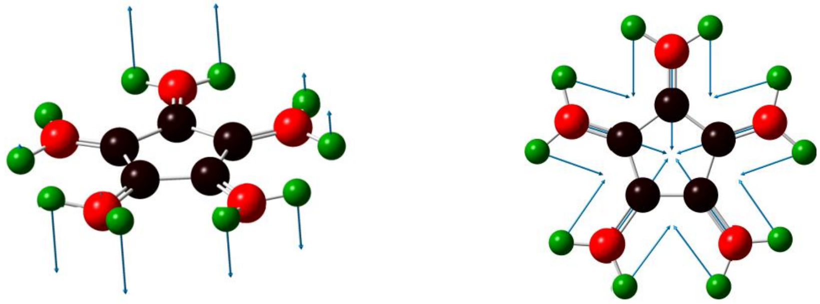
ν_{26}, **1709 cm^{-1}**
$\nu C=C$ stretching vibration

ν_2, **1503 cm^{-1}**
δCH_2 (scissoring) vibration



ν_3, **1503 cm^{-1}**
δCH_2 (scissoring) vibration

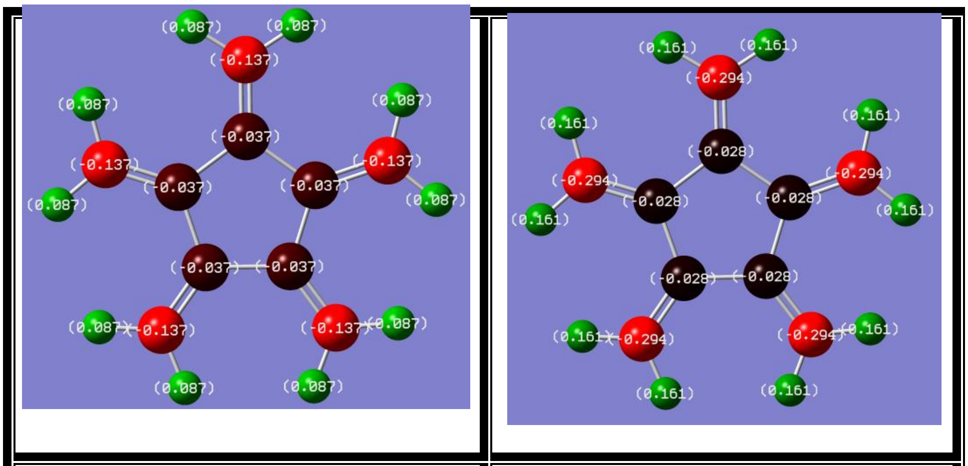
ν_{30}, **1268 cm^{-1}**
$\nu C\text{-}C$ stretching vibration



ν_{41}, **937 cm^{-1}**
γCH_2 (wagging) vibration

ν_4, **631 cm^{-1}**
δring (δCCC) breathing

Figure 3- Graphical pictures of some vibration modes for 5Radialene molecule as calculated applying the DFT method.



PM3			DFT (6-311G/ B3LYP)		
atom	**Electronic charge density**		**atom**	**Electronic charge density**	
-H	**0.087**	🟩	**H**	**0.161**	🟩
=C	**-0.137**	🟥	**=C**	**-0.294**	🟥
-C	**-0.037**	🟫	**-C**	**-0.028**	⬛

Figure 4- Distribution of electronic charge density at the atoms of 5Radialene molecule as calculated by semi-empirical method (PM3) and DFT (6-311G/ B3LYP) level methods.

4. Conclusion.

Application of the semiempirical PM3 and DFT (6-311G/ B3LYP) methods allowed a proper evaluation of all vibration frequencies of 5Radialene molecule. Our treatment provides complete assignment of all vibration modes (3N-6).The frequency values for the PM3 compared well with the DFT (6-311G/B3LYP) values. No experimental vibration frequencies are known.

Applying this computatively convenient methods allowed the valance assignment for the vibration modes of this molecule for the first time. The results allowed interesting relations between the different vibration modes and could be useful for the discussion of different problems of stability and reactivity of the molecule considered by the work.

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