Study of pyridyl and phenyl anellated imidazole-2-ylidenes and Si/Ge heavier analogues: structure, stability and aromaticity by DFT method

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Abstract

In this study, the structure, relative stability and aromaticity of structural isomers of imidazole-2-ylidene anodized by phenyl or pyridyl and their heavier Si and Ge companions were examined by DFT method. Also, NBO calculations were performed to obtain important information about a pair of unstable electrons, polarity, the charge on each atom, and the bonding order of the bonds in the molecule, the shapes of the molecular orbitals (HOMO and LUMO). NBO calculations were done on optimized structures using the rB3LYP computational method and in line with the command # POP = NBO (NBO, SAVE NBO) rB3LYP / 6-311 ++ G (3df, 3pd). The energy discrepancy of the HOMO and LUMO orbitals is the perturbation energy of the interaction between the natural giving and receiving orbitals obtained from NBO calculations. Hydrogenated reactions were also examined, as the results confirmed the findings on the energy stability of the optimized structures. NICS calculations were another case to be examined in the aromatic properties of the isomers. Based on the findings friom NICS calculations, N-heterocyclic carbon isomers have more aromatic properties than n-heterocyclic germline and silylene isomers.

Keywords: Stability, Carbon isomers, N-heterocyclic silylene and germylene, NBO calculations, Atomic charge, NICS calculations, DFT computational method

INTRODUCTION

Organic compounds are highly diverse. The main reason for this diversity is the way the atoms are placed next to each other. These atoms may be positioned in such a way to form a ring. Organic cyclic compounds also fall in two main types. If the ring formed contains only carbon atoms, it is called a homocycle, but if at least another element (S, N, O) is present in it in addition to the carbon, it is known as heterocycle. Compounds are also present in nature and are synthesized in the laboratory. One of the reasons why heterocyclic compounds are widely used is that their structure can be skillfully manipulated to meet the desired goals. Heterocyclic compounds today often work as optically active ligands and their complexes as catalysts in asymmetric synthetic reactions.

Heterocyclic compounds are largely distributed in nature. Many of which are of paramount significance in the living system. Many of the drugs and other major heterocyclic compounds with practical applications are not extracted from natural sources (due to the difficulty in making very small quantities), rather they are made. Despite the importance and level of heterocyclic compounds, heterocyclic compounds contribute significantly to biological processes, hence scientists seek to understand the chemistry of heterocyclic compounds to strengthen the quality of human life [1-3].

Because of the similarity of silicon and germanium, these two atoms have been examined in parallel with carbon. Ardengo et al. concluded that the electron density distribution of silylenes and germinins were substantially different from their companion carbons, and, they are like the Group 14 element, with a DAB ligand. This is while, a large number of calculations performed in different studies, directly led to the conclusion that silylenes and germylene were stabilized by the non-establishment of $p\pi$-$p\pi$ [4].

All chemists make use of models to better understand chemical problems. Molecular mechanics simulators apply the classical physics laws to predict the structure and

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properties of the molecules and to perform the calculations based on the nuclei interaction. This is while electronic structure techniques are based on quantum mechanics laws.

Computational chemistry results complement the data obtained from experimental methods and chemical experiments and can even lead to predicting unobserved chemical phenomena. In other words, computational chemistry serves as a laboratory and can compete with laboratory chemistry to find new issues in chemistry. On the other hand, the compounds studied in this study have not been synthesized in abundance as they have remained unstable in the laboratory; this is when there are interesting structural points about them making them be further examined.

Typically, their heterocyclic compounds and carbons were studied in laboratories, despite nitrogen, oxygen, and sulfur atoms. A comparison of the results from practical work and theoretic results as well as replacement of these atoms with more atoms such as silicon and germanium can yield valuable information on these compounds.

In this study, the stability energy of optimized structures and the level of aromatic property are considered as the most important parameters to measure the level of stability of carbon structural isomers, germylene and n-heterocyclic silylene. The energy discrepancy between HOMO and LUMO orbitals and the way NBO charge is distributed on the three atoms were calculated as two factors affecting the length of the carbon-heteroatom bond in the isomers.

MATERIALS AND METHODS
Basic sets
A basic set is a set of alternative mathematical functions to solve the Schrödinger 's time-independent equation for multi-electron systems, that can be provided by approximation numerical methods. Usually, the more the basic method and set used, the more accurate and realistic our calculations will be, but more time is to be spent on the calculation.

Basic methods
Computational chemistry calculations can be divided into the following four general categories:
1. Molecular mechanics method
2. Semi-experimental method
3. Ab initio.
4. Density functional theory

Density Funtional Theory (DFT) Method
Energy is an n-electron system that can be expressed in terms of the electron probability density; in other words, energy is written as energy density $(\rho)\varepsilon$ and density as ρ (r). Put it differently, density is a function of spatial coordinates [5]. In the DFT method, the electron energy obtained is written as follows:

εT refers to the kinetic energy stabilized by the electrons motion, εV refers to the potential energy that involves the nucleus-electron interaction. εJ is the electron-electron repulsive energy and finally εXC is the correlative energy and an exchange of electrons.

The term εXC involves two types of energy:
1. Quantum quantum mechanical energy related to the electron spin
2. Dynamic correaltive energy related to the electron motion

Software
Gaussian Software 01
The principal software applied in this research work is Gaussian software. Calculation of molecular and structural energy, energy and structure of the transition state, vibrational frequencies, thermochemical properties, reaction energy, reaction path, molecular orbitals, atomic charges, etc. are included in the possibilities provided by this software. The calculations done by the Gaussian 03 program can be performed in the gas phase and in solution, as they can also be related to the ground and excited states.

Gauss View Software 5
Gauss View is a graphical user' interface that helps manage the input monitor and control the graphical output Gaussian view produces.

Optimization
In this research, the # OPT B3LYP / 6-311 + G* method was used to optimize the structures.

All calculations in this study were performed by the Gaussian software 03 as the geometric structure of structural isomers of imidazole-2-ylide anodized by phenyl or pyridyl and their heavier Si and Ge companions was optimized by DFT method. In order to examine the thermodynamic stability of these structural isomers, frequency calculations were done on these isomers optimized by the DFT method with their zero-point energy computed.

Frequency calculations
Frequency calculations in this study were done by the command # FREQ=NO RAMAN HF/6-31G(d) Energy calculations

Energy calculations were performed to obtain the exact energy of the optimized structures by #ENERGY OPT rB3L YP/6-31G(d) method in the gas phase.

Corrected Zero Point Energy (ZPE)
ZPE is an inherent and intramolecular property. Its formula for all molecules is as follows:

$$ZPE = (1/2) \Sigma h\nu i$$

$$\varepsilon = \varepsilon_T + \varepsilon_V + \varepsilon_J + \varepsilon_{XC}$$

In this relation, vi represents usual frequencies in a molecule and h is Planck constant.

Dihedral angles

All dihedral angles in all of the nine isomers are equal to 0 or 180 degrees, suggesting that the carbon isomers are flat.

NBO (Natutal Bond Orbital) calculations

NBO calculations provide the researcher with important information concerning a pair of unstable electrons, the charge transfer energy, atoms hybridization in each bond of the molecule, the charge on each atom, and the bond order of the various bonds in the molecule. The atomic charge obtained by the NBO method is the most reliable type of computational atomic charge. The atomic charge is obtained by NBO calculations on structures optimized by the rB3LYP computational method and by the greatest baseline set according to the command POP = NBO (NBO, SAVE NBO) rB3LYP / 6-311 ++ G (3df , 3pd).

Polarity

After optimizing the geometric structures of carbon series isomers, silylene and germylene of NBO calculations were used to determine the degree of polarity of these isomers.

NICS (Nuleus-Independent Chemical Shift) calculations

In this study, the command # NMR rB3LYP/6-311++G(3df,3pd) was used to calculate the NICS. If these calculations are performed at a distance of 1 angstrom above or below the intended loop, it is represented by NICS (1). NICS (1) is used more to determine the aromatic property because NICS (1) can better reflect the effect of π electrons. NICS calculations are performed to examine the cause of stability. In literature review, it has been frequently stated that aromatic compounds enjoy more stability.

The structure of the studied isomers
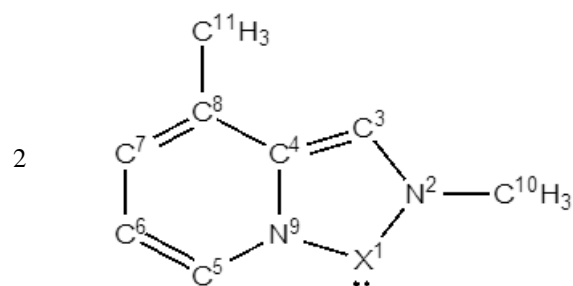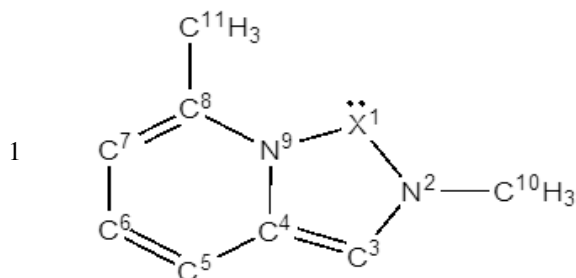
(X: C, Ge, Si)
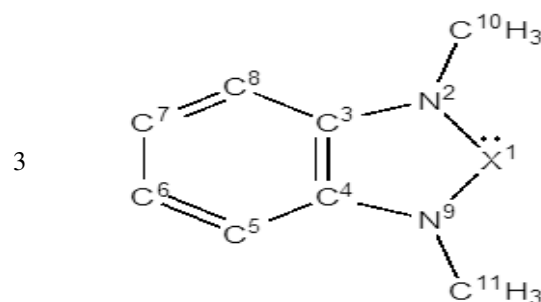
RESULTS

Energy calculations

In Table (1) Energy, the energy differences relating to the structural isomers of carbon, and N-heterocyclic silylene and germylene in the gas phase are collected by the DFT method in terms of kilocalories per mole. In the DFT method, the third isomer has more stability in each series of isomers, hence that the stability of isomers in each series of isomers is as follows:

3a > 2a > 1a
3b > 2b > 1b
3c > 2c > 1c

A comparison between the carbon isotherms series, and N-heterocyclic silylene and germylene, stable N-heterocyclic, isomers of n-heterocyclic germylene series are greater than silylene isomers of N-heterocyclic and N-heterocyclic carbon isomers and the order of stability of these three series is as follows:

NHGes > NHSis > NHCs

The stability of the third isomer in each isomers series is due to the greater symmetry of the third isomer than the other isomers in the series, and this stability represents the reality on the ground that the more symmetrical the compound, the more stable it is.

The stability of the N-heterocyclic germylene isomers series with respect to the silylene series and carbon ions is due to the properties of the Ge atom with respect to Si and C, and the higher stability of the silylene isomers series with respect to the carbon series is due to this Si atom property.

Table 1: Optimized energy of structural carbon, N-heterocyclic silylene and germylene isomers by DFT method

Structure	E_{opt} (kcal mol^{-1})	ZPE (kcal mol^{-1})	E_{opt} + ZPE
	DFT		
1a	-287662.9	116.1	-287546.8
2a	-287662.5	116.2	-287546.3
3a	-287676.0	116.4	-287559.6
1b	-1565862.6	112.9	-1565749.7
2b	-1565860.1	113.0	-1565747.1
3b	-1565874.8	113.3	-1565761.5
1c	-445455.9	113.2	-445342.7
2c	-445454.9	113.3	-445341.6
3c	-445470.4	113.8	-445356.6

Frequency calculations

The results from frequency calculations by DFT method are provided in Table (2) and the vibration frequency order of carbon series isomers is as follows:

3a > 1a > 2a method DFT

The vibrational frequencies order of germylene series isomers is as follows:

3b > 2b > 1b

method DFT

The vibrational frequencies order of silylene series isomers is as follows:

3c > 2c > 1c
method DFT

A comparison of the carbon series, germylene and n-heterocyclic silylene shows that the vibrational frequencies of N-heterocyclic carbon isomers is greater than the vibrational frequency of N-heterocyclic silylene and the vibrational frequency of N-heterocyclic silylene is greater; this is while, the order of the values of the first vibration frequency of the isomers is as follows:

NHCs > NHSis > NHGes

Table 2: The first vibrational frequency of structural isomers of carbon, and N-heterocyclic silylene and germylene by DFT method in terms of v (cm^{-1})

Structure	DFT
1a	178.3581
2a	178.2991
3a	191.2573
1b	118.8676
2b	121.2143
3b	141.4011
1c	145.7053
2c	146.8502
3c	165.4840

Data in Table (2) suggest that in the DFT method, the first vibration frequency of all isomers has a positive value, indicating the stability of these compounds and the correctness of the optimization calculations.

Length of the bond

The order of the carbon bond lengths values in the N-heterocyclic carbon isomers series is as follows:

2a > 1a > 3a method DFT

According to the findings, it can be explained that there is an interaction between the single pair of nitrogen atoms and the near empty p orbitals of carbon, silylene and germylene. There is more evidence for this interaction, such as UV-vis spectra, NBO charges, and also electrophilic and nucleophilic properties.

The length values order of germylene bonds in N-heterocyclic germylene isomers by the DFT method is as follows:

1b > 2b > 3b

However, the difference of values in bond length between these isomers is insignificant, and isomers 1b and 2b have approximately an equal bond lengths. The order of the length values of silylene bonds in N-heterocyclic silylene isomers in the method used is as follows:

1c > 2c > 3c method DFT

Table 3: Length values of carbon, germlyne and silylene bonds in carbon, germlyne and N-heterocyclic isomers in the gas phase by DFT method based on angstrom (X: C, Ge, Si)

Structure	DFT	
	$X^1 - N^2$	$X^1 - N^9$
1a	1.365	1.384
2a	1.366	1.385
3a	1.374	1.374
1b	1.892	1.912
2b	1.885	1.906
3b	1.872	1.872
1c	1.779	1.821

2c	1.776	1.813
3c	1.773	1.773

Bond angles

Table (4) illustrates the bonding angles of the isomers via the DFT method.

Table 4: Bonding angles of carbon, and N-heterocyclic silylene and germylene isomers in gas phase by DFT method in terms of degrees (X: C, Ge, Si)

Structure	Bond angle (°)	DFT
1a	N^9- C^1- N^2	100.84
2a	N^9- C^1- N^2	100.62
3a	N^9- C^1- N^2	102.98
1b	N^9- Ge^1- N^2	82.58
2b	N^9- Ge^1 -N^2	82.64
3b	N^9- Ge^1 -N^2	84.85
1c	N^9- Si^1 -N^2	85.54
2c	N^9- Si^1 -N^2	85.44
3c	N^9- Si^1 -N^2	87.80

Dihedral angles

The dihedral angles values of the isomers in all the nine isomers are equal to 0 or 180 degrees, indicating that the carbon isomers are flat and as a result these cyclic isomers become aromatic.

Polarity

NBO calculations are used to determine the polarity of the isomers. According to Table (5), the dipole moment of N-heterocyclic carbon isomers is greater than the dipole moment of N-heterocyclic silylenbe and germylene isomers. The order based on which the dipole moment increases is as follows:

NHCs > NHSis > NHGes

The dipole moment values of these three isomers series indicate that the N-heterocyclic carbon isomers have greater polarity than the N-heterocyclic silylene and germylene isomers. N-heterocyclic silylene isomers are more polar than N-heterocyclic germylene isomers.

According to the data in Table 5, one can conclude that the more symmetric the molecule, the lower the polarity, and the more asymmetric the molecule, the higher the polarity.

In N-heterocyclic carbon series isomers, the second isomer 2a has more polarity than the other isomers in this series, and isomer 3a, being more symmetrical than the other two isomers in this series, has less polarity than the other two isomers. The order of polarity of the N-heterocyclic carbon series isomers is as follows:

2a > 1a > 3a

According to the data in Table (5) in the N-heterocyclic germylene isomers seris, isomer 2b has more polarity, indicating that the structure of this isomer is less symmetric than other isomers in this series. The lowest degree of polarity in this series belongs to isomer 3b because of the more symmetrical structure of this isomer than other isomers in this series. The order of polarity in the N-heterocyclic germline isomers series is as follows:

2b > 1b > 3b

According to Table 5, in the N-heterocyclic silylene isomers series, the polarity of isomer 2c is greater than that of the other two isomers, and this polarity stems more from the asymmetric structure of molecule 2c.

Table (5) does not illustrate the dipole moment value for isomer 3c; the NBO calculations of this isomer face an error.

It should be stated that all isomers studied have a point group of C1.

Table 5: Dipole moments of carbon, germylene and silylene series isomers by DFT method

Structure	Dipole moment	Point group
1a	1.87	C1
2a	2.89	C1
3a	1.71	C1
1b	0.90	C1
2b	1.54	C1
3b	0.64	C1
1c	1.08	C1
2c	1.78	C1

NBO Analysis

To examine inter-molecular hydrogen bonding, attention is focused on stability energy, where this energy is calculated by the second-order perturbation theory analysis of complexes relating to electron pairs in only one of the atoms and the anti-bonding orbital in the other atom, connected to a hydrogen bonding. In this way, the perturbation energy will be a measure of the strength of the hydrogen bonding. Table (6) illustrates the perturbation energy of all the isomers studied. According to Table (6), isomer 2b has the greatest perturbation energy, enjoying a perturbation energy of 243.20 kcal/mmol.

Table 6: Perturbation energy of the interaction between the natural giving and receiving orbitals

Strcuture	(i) NBO giving	Receiving (j) NBO	E (kcal mol^{-1})
1a	LP (1) N_{20}	BD* (2) N_{19} - C_{21}	49.68

2a	LP (1) N_{19}	BD* (2) N_{20} - C_{21}	47.08
3a	LP (1) N_{20}	LP* (2) C_7	95.99
1b	LP (1) N_{20}	BD* (2) C_1 - C_6	39.35
2b	LP (1) C1	BD* (2) C_6 - N_{20}	243.20
3b	LP (2) Ge_{11}	BD* (2) C_1 - N_{20}	13.90
1c	BD (2) N_{12} -Si_{21}	LP (1) C_1	53.23
2c	LP (1) N 19	LP* (2) Si_{21}	141.46
3c	LP (1) C_1	BD* (2) C_2 - N_{19}	212.67

Energy difference for HOMO and LUMO orbitals

When creating a bond between two atoms, their atomic orbitals overlap each other to form molecular orbitals. In wave function chemistry, molecular orbital determines the energy level of the electrons of a molecule. Molecular orbitals are divided into two bonding and anti-bonding types. In chemistry, in terms of the energy level of molecular orbitals, the highest molecular orbital is known as HOMO and the lowest electron-free molecular orbital as LUMO. Table (7) illustrates the energy differences of HOMO and LUMO orbitals for structural isomers of carbon, and N-heterocyclic germylene and silylene. As you can see in this table, isomer 1a has the greatest level of energy difference between HOMO and LUMO orbitals and isomer 1b has the lowest amount of energy difference between HOMO and LUMO orbitals, creating stability for isomer 1a compared to other isomers.

**Table 7:** Energy difference of HOMO and LUMO orbitals in terms of Kcalmol-1

| Compound	HOMO	LUMO	HOMO-LUMO (Kcal/mol)
1a	-0.19734	-0.4239	142.17
2a	-0.19999	-0.04415	-97.79
3a	-0.22717	-0.03262	-122.08
1b	-0.16284	-0.04933	-71.23
2b	-0.16365	-0.04861	-72.19
3b	-0.20115	-0.05782	-89.94
1c	-0.17100	-0.04490	-79.13
2c	-0.17216	-0.04264	-81.27

Hydrogenation reactions

In Table (8), the hydrogenation energy reactions of structural isomers are examined and their relative energies are gathered. According to Table (8) and comparing the three isomers series, the N-heterocyclic carbon series isomers have been found to be more stable by hydrogenation reaction than the N-heterocyclic silylene and germylene isomers. The order of stability the studied isomers in hydrogenation reactions is as follows:

NHCs-H > NHSis-H > NHGes-H

Also, according to Table (8), in N-heterocyclic carbon isomers, isomer 3a is more stable than the other two isomers in the hydrogenation reaction. The order of stability of N-heterocyclic carbon isomers in the hydrogenation reaction is as follows:

3a > 2a > 1a
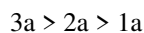
In N-heterocyclic germylene series isomers, isomer 3b is more stable than the other two isomers in the hydrogenation reaction. The order of stability of N-heterocyclic germylene isomers in the hydrogenation reaction is as follows:

3b > 2b > 1b
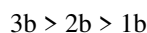
In N-heterocyclic silylene series isomers, isomer 3c is more stable in the hydrogenation reaction than the other two isomers. The order of stability of N-heterocyclic silylene series isomers in the hydrogenation reaction is as follows:
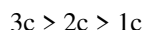
3c > 2c > 1c

Table 8: Energy and relative energy of hydrogenation reactions of structural isomers under study

Strstructure	Reactor energy		Energy is the main product of the hydrogenation reaction	Reaction energy	Reaction energy (Kcal mol^{-1})	Relative energy
	Isomers	H$_2$				
1a	-458.42701604	-1.175	-459.63206999	-0.03005395	-18.8	-10.5
2a	-458.42631045	-1.175	-459.63193955	-0.0306291	-19.2	-10.1
3a	-458.44789585	-1.175	-459.66958345	-0.0466876	-29.3	0
1b	-2495.39855100	-1.175	-2496.54419979	0.02935121	18.4	-8.6
2b	-2495.39465675	-1.175	-2496.54154027	0.02811648	17.6	-7.8
3b	-2495.41798608	-1.175	-2496.57728563	0.01570045	9.8	0
1c	0.02935121	-1.175	-711.07329136	-0.00845738	-5.3	-8.5
2c	0.02811648	-1.175	-711.07239871	-0.00915342	-5.7	-8.1
3c	0.01570045	-1.175	-711.11008040	-0.02202464	-13.8	0

NICS calculations

According to the results of these calculations, the loops with negative numbers are aromatic and non-aromatic compounds have a NICS number close to zero and anti-aromatic compounds with a positive NICS number. NICS calculations are usually performed at the center of the loop, which is represented by NICS (0). However, these calculations can also be done at a certain distance from the top or bottom of the center of the loop. If these calculations are performed at a distance of .0.5 Å above or below the intended loop, it is performed with NICS $_{(0.5)}$ and if these calculations are performed at a distance of Å 1 higher or lower than the intended loop, it is specified by NICS (1) (Table 9).

NICS (1) tends to be used more to determine aromatic properties because NICS (1) can better reflect the effect of π electrons. As well, NICS $_{(1)}$ $_{ZZ}$ calculations include calculations performed at a distance of Å 1 above or below the loop and along the Z axis, which yield better NICS (1) and NICS $_{(1)ZZ}$ calculations among the NICS. For example, NICS calculations performed at a distance of Å 1 above the center of benzene and phenol loops are -10.1 and -9.6 ppm, respectively. In Table (9), NICS $_{(0)}$, NICS $_{(0)}$ $_{ZZ}$, NICS $_{(0.5)}$, NICS $_{(0.5)}$ $_{ZZ}$, NICS $_{(1)}$, NICS $_{(1)}$ $_{ZZ}$ calculations of quintuple and hexagonal loops of carbon isomers, N-heterocyclic germylene and silylene are well shown. As said, it is better to use NICS $_{(1)}$ $_{ZZ}$ calculations to compare and determine aromatic properties. From among of N-heterocyclic carbon series isomers, the quintuple loop isomers (1a) has NZS $_{(1)}$ $_{-ZZ}$ = 35.17, which have more aromatic properties compared to the 5-loop seris isomers with the values of -0.33 and -2.99 ppm, respectively. Among the other two isomers in this series, isomer (2a with 33.07 ppm) has more aromatic property than isomer (3a).

The order of increasing the aromatic character of the 5-loop N-heterocyclic carbon isomers is as follows:

(1a) > (2a) > (3a)

The order of aromatic properties of this series isomers of for the 6-loop isomers are as follows: isomer (3a) with the value -30.70 ppm is greater than the other two isomers with the value of -13.78 and -13.16 and isomer (1a) with the value 13.78 ppm - NICS (1) ZZ = is more aromatic than isomer (2a) with ppm number 13.16- NICS (1) ZZ =.

The order of increasing the aromatic character of the 6-loop of N-heterocyclic carbon series isomers is as follows:

(3a) > (1a) > (2a)

Comparison of NICS numbers of 5- and 6-loops yielded higher values of NICS for 5-loops than 6-loops in two isomers (1a) and (2a). That is, in the N-heterocyclic carbon series isomers of a 5-loop, it has a higher aromaticity than a 6-loop isomner, which may be due to the presence of electron pairs on the nitrogen atoms in it.The order of increasing the aromatic properties of the 5 and 6 isomer loops of each series with their counterparts in the other series is as follows:

F loops

(1c)   (1b) > (1a) >

(2a) > (2b) > (2c)

(3a) > (3b) > (3c)

6 loops

 (1c)   (1b) > (1a) >

(2a) > (2c) > (2b)

(3a) > (3c) > (3b)

In general, the following result can be obtained from comparing numbers:

NHCS> NHGeS> NHSiS

Table 9 - Data obtained from NICS calculations by DFT method

		Five loops	Six loops
	NICS 0	-14.55	-3.31
	NICS 0.5	-15.59	-4.56
1a	NICS 1	-12.65	-5.27
	NICS 0(ZZ)	-16.88	+4.97
	NICS 0.5(ZZ)	-31.19	-3.87
	NICS 1(ZZ)	-35.17	-13.78
	NICS 0	-13.69	-3.44
	NICS 0.5	-14.66	-4.64
2a	NICS 1	-12.00	-5.26
	NICS 0(ZZ)	-14.25	+5.51
	NICS 0.5(ZZ)	-28.45	-3.27
	NICS 1(ZZ)	-33.07	-13.16
	NICS 0	-9.19	-10.63
	NICS 0.5	-10.53	-11.79
3a	NICS 1	-9.27	-11.18
	NICS 0(ZZ)	+0.33	-16.96
	NICS 0.5(ZZ)	-13.05	-25.18
	NICS 1(ZZ)	-21.99	-30.70

		Five loops	Six loops
	NICS 0	-13.17	-1.28
	NICS 0.5	-13.04	-2.62
1b	NICS 1	-10.61	-3.74

	NICS 0(ZZ)	-9.43	+10.06
	NICS 0.5(ZZ)	-20.32	+1.05
	NICS 1(ZZ)	-27.82	-9.75
	NICS 0	-10.94	-0.79
	NICS 0.5	-11.14	-2.11
2b	NICS 1	-9.36	-3.07
	NICS 0(ZZ)	-6.08	+12.88
	NICS 0.5(ZZ)	-17.46	+3.40
	NICS 1(ZZ)	-25.49	-7.77
	NICS 0	-8.76	-9.37
	NICS 0.5	-8.96	-10.71
3b	NICS 1	-7.57	-10.38
	NICS 0(ZZ)	+5.42	-14.69
	NICS 0.5(ZZ)	-5.29	-22.84
	NICS 1(ZZ)	-16.08	-28.68

		Five loops	Six loops
	NICS 0	-11.76	-1.22
	NICS 0.5	-12.12	-2.44
1c	NICS 1	-9.96	-3.48
	NICS 0(ZZ)	-10.65	+10.74
	NICS 0.5(ZZ)	-21.66	+1.77
	NICS 1(ZZ)	-27.81	-9.02
	NICS 0	-9.84	-0.86
	NICS 0.5	-10.26	-2.13
2c	NICS 1	-8.75	-3.19
	NICS 0(ZZ)	-6.25	+12.12
	NICS 0.5(ZZ)	-17.52	+3.24
	NICS 1(ZZ)	-24.66	-7.68
	NICS 0	-7.62	-9.50
	NICS 0.5	-7.98	-10.81
3c	NICS 1	-6.80	-10.43
	NICS 0(ZZ)	+4.80	-14.84
	NICS 0.5(ZZ)	-5.18	-22.97
	NICS 1(ZZ)	-14.70	-28.77

CONCLUSION

In this study, three structural isomers series of carbon, and N-heterocyclic germylene and silylene were examined using Gaussian software 03. According to the results from energy calculations, the stability of N-heterocyclic germylene isomers is greater than N-heterocyclic silylene isomers and N-heterocyclic silylene isomers are greater than N-heterocyclic carbon isomers, and the order of stability can be stated as follows:

NHGes > NHSis > NHCs

We also found out that the third isomer of each series was more stable than the other two isomers of that series, and this validates the rule that the more symmetric the compound, the more stable it is.

Based on the calculations, there is a high correlation for the non-bonded pair of nitrogen alone for the interaction of the empty P orbital of the divalent centers of carbon, xylene and germylene in a single state. There is evidence for UV-Vis spectra, NBO charge, and electrophilic and nucleophilic properties for this interaction. Bivalent centers are very electron-friendly.

The atomic charge of the N atom is negative because it involves a single electron pair and the carbon atomic charge is negative because it involves two electrons on it, however the N atom is found to be more negative, creating more interaction between the electrons of the N atom and the empty orbitals of the atoms. According to the calculations done and examination of dihedral angles, these 9 isomers are flat structurally and as a result these cyclic isomers can be aromatic. According to NICS calculations, symmetry increases the resonance property and thus the aromatic property.

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