

NBO and QTAIM investigations of the conformers of 1, 4-dioxane-2, 3-bis(pyridin-1-ium) and 1, 4-dioxane-2, 5-bis(pyridin-1-ium) molecules

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Abstract

This research aimed at exploring the stabilities of conformers of 1, 4-dioxane-2, 3-bis(pyridin-1-ium) and 1, 4-dioxane-2, 5-bis(pyridin-1-ium) molecules at the B3LYP/6-311+G (d,p) theory level. To this goal, estimations of the total energies and dipole moments of the *axial* and *equatorial* conformations were first done for the mentioned molecules. C-N and C-O bond distances were calculated and these variations were explained with the negative hyperconjugative anomeric effects. The negative hyperconjugative anomeric effect on the axial conformer was illustrated by NBO analysis and the interactions responsible for the effect were explored. Also, QTAIM study was used for illustration of the C-N and C-C bonds in the studied systems.

Keywords: 1, 4-Dioxane; negative hyperconjugative effect; conformers; natural bond orbital analysis (NBO); quantum theory of atoms in molecules (QTAIM).

Introduction

1, 4-Dioxane is a heterocyclic organic compound that is classified as an ether. This colorless liquid has a faintly sweet odor similar to that of diethyl ether. The compound is often called simply dioxane because the other dioxane isomers (1, 2- and 1, 3-) are rarely encountered. Dioxane is used as a solvent for a variety of practical applications as well as in the laboratory, and also as a stabilizer for the transport of chlorinated hydrocarbons in aluminum containers [1,2]. Since 1,4-dioxane is a probable human carcinogen and is highly miscible in water [1], special attention has been given to its

presence in subsurface aquifers where it poses a health risk. Synthesis and properties of various compounds of the family of 1,4-dioxane molecules have been investigated in several studies [3-11].

The synthesis of 2,3-dichloro- and 2, 3-dibromo-1, 4-dioxanes [12] and also 2, 5-dichloro-1, 4-dioxane [13] molecules has been reported and the geometry and conformations of these compounds have been accurately determined using X-ray diffraction (XRD) techniques [14]. The obtained results demonstrated the existence of only the axial-axial conformation in this compound and showed that the endocyclic atomic

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distances from oxygen atom to a carbon atom carrying a halogen atom are significantly smaller than the corresponding distances to carbon atoms without halogen atoms. Also, the structure and spectroscopic properties of dioxanylamine have been studied [15-17].

The stability of the conformation in the many cyclic molecules is influenced with the anomeric effect [18]. The anomeric effect is occurred when two electronegative substituents are attached to a sp^3 -hybridized carbon atom. Computational studies are useful for explanation of the anomeric effect in the cyclic molecules the same as what have been employed to illustration of the structure and properties of the molecules [19-28]. Numerous theoretical investigations have been reported about the anomeric effect [29-41].

In the present investigation, the stabilities of conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) and 1,4-dioxane-2,5-bis(pyridin-1-ium) are studied at the B3LYP /6-311+G(d,p) theory level. In addition, the negative hyperconjugative anomeric effects of these conformers are explored by NBO analysis. Also, QTAIM study was employed for illustration of the C-N and C-C bonds in the studied systems.

Computational methods

All computations were carried out with the Gaussian 09 software package [42]. The calculations were carried out using standard 6-311+G(d,p) basis set [43-45]. The B3LYP hybrid functional method

was utilized to optimize the geometries [46-48]. B3LYP uses the non-local correlation provided by the LYP expression.

The characteristics of each observed stationary point have been confirmed in terms of having the least energy by conducting a vibrational analysis. In this regard, Gaussian 09 software suite is employed to analyze the population through the NBO process of the NBO 6.0 program [49] at the B3LYP/6-311+G(d,p)theory level.

Quantum theory of atoms in molecules analysis (QTAIM) computations were performed with the Multiwfn 3.5 package [50].

Results and discussion

Energetic aspects

Conformers of the *axial* and *equatorial* conformers of 1, 4-dioxane-2, 3-bis(pyridin-1-ium) and 1, 4-dioxane-2, 5-bis(pyridin-1-ium) molecules are depicted in Figure 1. The absolute energy and relative energy values of these conformers are gathered in Table 1. As can be seen, the *axial* conformer is more stable than *equatorial* conformer in both isomers. Moreover, more relative energy values ($\Delta E(1)$) of equatorial conformer in II-isomer can be observed compared to I-isomer.

On the other hand, energetic aspect shows the more stability of II-isomer than I-isomer. The corresponding relative energy values ($\Delta E(2)$) are larger in equatorial conformer compared to axial isomer.

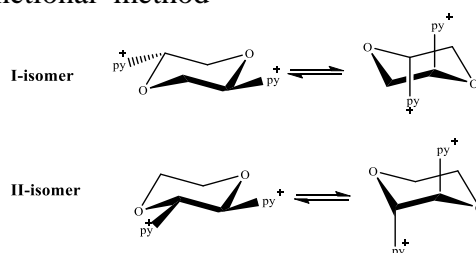


Figure 1. *axial* and *equatorial* conformers of 1, 4-dioxane-2, 3-bis(pyridin-1-ium) (I) and 1, 4-dioxane-2,5-bis(pyridin-1-ium) (II) molecules

Table 1. Absolute energy (a.u), relative energy (kcal/mol) and dipole moment (μ , Debye) values of the *axial* and *equatorial* conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) (**I**) and 1,4-dioxane-2,5-bis(pyridin-1-ium) (**II**) molecules at B3LYP/6-311+G(d,p) level of theory

isomer	E		$\Delta E(1)$		$\Delta E(2)$		μ	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	-802.681	-802.681	0.44	0.00	7.35	11.10	2.4949	4.2807
II	-802.692	-802.699	4.19	0.00	0.00	0.00	0.00	0.00

Molecular orbital analysis

The energies of the frontier orbitals (HOMO, LUMO), the corresponding HOMO–LUMO energy gaps, hardness, chemical potential and electrophilicity values of the investigated molecules are given in Table 2.

According to the Koopmans' theorem, ionization potential (IE) and Electron affinity (EA) values are:

$$IE = -E(\text{HOMO}); EA = E(\text{LUMO})$$

Therefore, chemical hardness (η), chemical potential (μ) and global electrophilicity index (ω) values can be calculated as:

$$\eta = \frac{E(\text{LUMO}) - E(\text{HOMO})}{2}$$

$$\mu = \frac{E(\text{LUMO}) + E(\text{HOMO})}{2}$$

$$\omega = \frac{\mu^2}{2\eta}$$

As shown in Table 2, HOMO–LUMO gap and hardness of *axial* conformer are more than *equatorial* conformer. As expected from the

minimum energy principle (MEP), and maximum hardness principle (MHP), that is, while a conformer changes from the most stable to other less stable species in most cases, the energy increases, and the hardness decreases [51-55].

The calculated electrophilicity (ω) values are listed in Table 2. The smaller ω values in *axial* conformer compared to *equatorial* conformer can be observed. This trend is compatible with the minimum electrophilicity principle (MEIP) [56,57] that is, while a conformer changes from the most stable to other less stable species in most cases, the energy increases, and the electrophilicity increases. This principle may be defined as, “electrophilicity will be a minimum (maximum) when both chemical potential and hardness are maxima (minima)”. The calculated chemical potential (μ) values of the studying molecules are shown in Table 2. It can be found, μ values of *axial* conformer are smaller than *equatorial* conformer.

Table 2. Absolute energy (a.u), relative energy (kcal/mol) and dipole moment (μ , Debye) values of the *axial* and *equatorial* conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) (**I**) and 1,4-dioxane-2,5-bis(pyridin-1-ium) (**II**) molecules at B3LYP/6-311+G(d,p) level of theory.

Molecule	E(HOMO)	E(LUMO)	Gap	η	μ	ω
<i>axial</i>						
I	-14.87	-9.45	5.43	2.71	-12.16	27.25
II	-14.87	-9.22	5.65	2.82	-12.04	25.69
<i>equatorial</i>						
I	-14.44	-9.62	4.82	2.41	-12.03	30.04
II	-14.42	-9.06	5.36	2.68	-11.74	25.70

Dipole moment

Generally, it has been accepted that there is a preference for the conformation with the smallest resultant dipole moment [58]. In the gas phase or in the nonpolar media, the conformations with the larger dipole moment may have the larger electrostatic energy. Therefore, we may expect that the conformation with the larger dipole moment may have greater overall energy. The calculated dipole moments for the *axial* and *equatorial* conformers investigated compounds are given in Table 1. These results show that the dipole moments for the *axial* conformer of the studied compounds are smaller than those in *equatorial* conformer. Orientations of the dipole moment vector are presented in Figure 2.

Structural parameters

C-N and C-O bond distances of the studied molecules are listed in Table 3. The comparison of the C-N bond distances shows the longer bonds in *axial* conformer compared to *equatorial* conformer. This variation in bond distances and the more stability of *axial* conformer compared to *equatorial* conformer are attributed to negative

hyperconjugation effects. Figure 3 represents the responsible NBOs of the mentioned negative hyperconjugation interactions which is explained in terms of a dominant $LP(2)O \rightarrow \sigma^*(C-N)$ negative hyperconjugation interaction between a pair of non-bonded electrons on oxygen and the adjacent C-N bond in *axial* conformer. This interaction is the donation of electron density from a filled p-orbital of oxygen to a neighboring σ^* -orbital of the C-N bond. This phenomenon, which is a type of resonance, can stabilize the molecule. As a result, it causes an elongation of the σ -bond by adding electron density to its anti-bonding orbital.

The second order perturbation theory analyses of Fock matrix in NBO basis of the $LP(2)O \rightarrow \sigma^*(C-N)$ interactions in the *axial* and *equatorial* conformers of the studied molecules are calculated. These calculations show that E(2) values are 16.89 and 14.31 kcal/mol for **I** and **II**-isomers, respectively. As can be noticed, the stronger the interactions in the $LP(2)O \rightarrow \sigma^*(C-N)$, the more negative the hyperconjugation interaction in **I**- isomer than **II**- isomer.

Table 3. Absolute energy (a.u), relative energy (kcal/mol) and dipole moment (μ , Debye) values of the *axial* and *equatorial* conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) (**I**) and 1,4-dioxane-2,5-bis(pyridin-1-ium) (**II**) molecules at B3LYP/6-311+G(d,p) level of theory.

isomer	C1-N		C1-O	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	1.5211	1.4925	1.3835	1.3884
II	1.5179	1.4896	1.4037	1.4058

QTAIM

The findings obtained from calculations of QTAIM may also describe the C-N and C-C bonds in the studied systems.

Electron density

The C-N and C-O bonds in the studied systems are listed in Table 4. The calculations of QTAIM indicate that the more density of electron on bond critical point (BCP) of C-N bonds in the *equatorial* conformer is compared to

axial conformer. This trend is compatible with the larger C-N distances in the *axial* conformer than *equatorial* conformer. The calculations of QTAIM indicate that the less density of electron on bond critical point (BCP) of C-O bonds in *equatorial* conformer is compared to *axial* conformer. This trend is compatible with the shorter C-O distances in the *axial* conformer than *equatorial* conformer.

Laplacian of electron density

Table 4 indicates $\nabla^2\rho$ values of C-N and C-O bonds which are negative at related bond critical points (BCP), as it was observed for strong covalent interaction (interactions of shared).

Energy density

The total energy density (E) on bond critical point (BCP) of a bond is defined as:

$$E = G + V$$

Where, G and V are Lagrangian kinetic energy and Virial energy density, respectively.

Table 4 indicates that the energy density (H) has negative values at the BCP of C-N and C-O bonds. Therefore, there are shared interactions at these BCPs.

One can also use the $|V(r)| / G(r)$ ratio as another useful description. $|V(r)|/G(r) > 2$ is diagnostic of a "classical" covalent interaction [59]. The corresponding $|V(r)|/G(r)$ ratio values at the BCP of C-N and C-O bonds are listed in Table 4; The significant covalent interaction in the C-C and C-N bonds can be deduced.

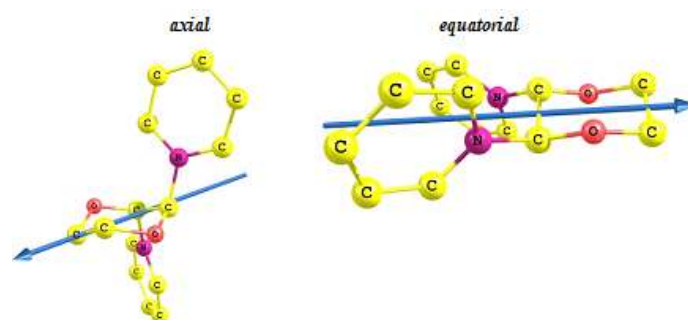


Figure 2. Orientations of the dipole moment vector are presented in *axial* and *equatorial* conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) molecules. Hydrogen atoms were omitted.

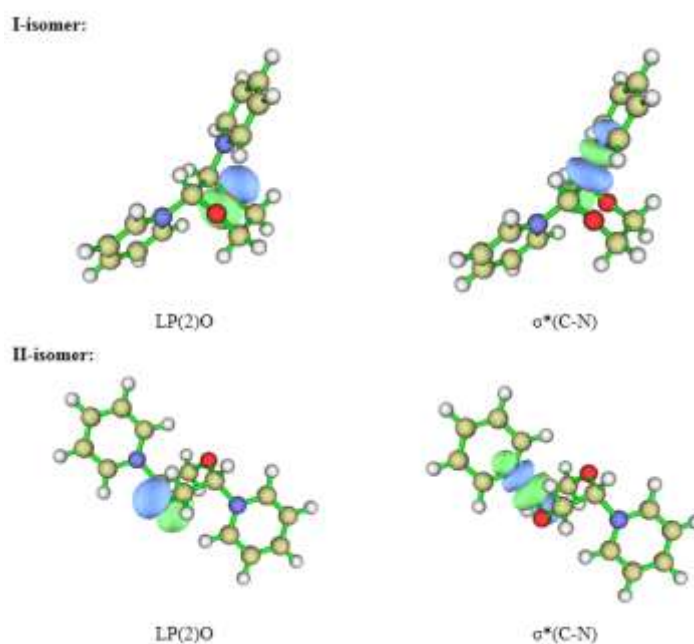


Figure 3. The responsible NBOs of the negative hyperconjugation interactions in terms of a dominant $LP(2)O \rightarrow \sigma^*(C-N)$ in *axial* conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) (I) and 1,4-dioxane-2,5-bis(pyridin-1-ium) (II) molecules

Table 4. QTAIM results of the bond critical point (BCP) of C-N and C-O bonds in the *axial* and *equatorial* conformers of 1,4-dioxane-2,3-bis(pyridin-1-ium) (**I**) and 1,4-dioxane-2,5-bis(pyridin-1-ium) (**II**) molecules at B3LYP/6-311+G(d,p) level of theory
(a) electron density (ρ , in e. \AA^3)

isomer	$\rho(\text{C1-N})$		$\rho(\text{C1-O})$	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	0.2322	0.2460	0.2276	0.2263
II	0.2326	0.2478	0.2712	0.2444

(b) Laplacian of electron density (ρ , in e. \AA^5)

isomer	$\nabla^2\rho(\text{C1-N})$		$\nabla^2\rho(\text{C1-O})$	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	-0.5293	-0.6285	-0.3370	-0.2878
II	-0.5382	-0.6421	-0.5876	-0.3869

(c) Lagrangian kinetic energy (a.u)

isomer	$G(\text{C1-N})$		$G(\text{C1-O})$	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	0.0962	0.1078	0.1970	0.2106
II	0.0993	0.1080	0.2148	0.2189

(c) Virial energy density (a.u)

isomer	$V(\text{C1-N})$		$V(\text{C1-O})$	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	-0.3247	-0.3728	-0.4782	-0.4931
II	-0.3332	-0.3766	-0.5765	-0.5345

(c) energy density (a.u)

isomer	$E(\text{C1-N})$		$E(\text{C1-O})$	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	-0.2285	-0.2650	-0.2812	-0.2825
II	-0.2339	-0.2686	-0.3617	-0.3156

(c) $|V(r)|/G(r)$

isomer	$E(\text{C1-N})$		$E(\text{C1-O})$	
	<i>axial</i>	<i>equatorial</i>	<i>axial</i>	<i>equatorial</i>
I	3.38	3.46	2.43	2.34
II	3.35	3.49	2.68	2.44

Abbreviations

NBO: Natural bond orbital analysis

QTAIM: Quantum theory of atoms in molecules

HOMO: Highest occupied molecular orbital

LUMO: Lowest unoccupied molecular orbital

MEP: Minimum energy principle

MHP: Maximum hardness principle

MEIP: Minimum electrophilicity principle

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