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Impact of gases on the planarity of alkyl-substituted α -oligofuran: DFT study

Joyanta K. Saha¹ · Jahir Raihan¹ · Mohammad Abdul Matin² · Joonkyung Jang³

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Abstract

By using the density functional theory, extensive calculations were performed at the M06-2X/6-311G(d,p) level of theory to assess the impact of different gaseous molecules (H₂O, CH₃OH, N₂H₄, H₂O₂, HCN, NH₃, SO₂, and CO₂) on the planarity of alkyl-substituted α -oligofurans (AOF). Of the eight gases, the greatest planarity distortion of AOF was observed with H₂O (*P*=0.88), CH₃OH (*P*=0.91), CO₂ (*P*=0.93), SO₂ (*P*=0.94), and H₂O₂ (*P*=0.94) when interacting with AOF on ring 1. When the gases interacted with AOF on ring 2, the planarity remained unchanged. The gases that disrupt the planarity of AOF exhibited a stronger interaction with AOF on ring 1 compared to ring 2. A natural bond orbital (NBO) analysis was conducted to examine the interactions between the gases and AOF on rings 1 and 2. The non-covalent interaction (NCI) analysis revealed that weak van der Waals interactions between Furan rings and alkyl chains in isolated AOF maintain their planarity. These interactions remain uninterrupted when the gases interact with ring 2 of AOF, thus preserving its planarity. However, when the gases interacted with ring 1 of AOF, the van der Waals interactions were disrupted, resulting in a distortion of the planarity.

Keywords Oligofurans · Planarity · NCI analysis · Conducting polymer · Dihedral angle

Introduction

Conductive polymers (CPs) [1] play a vital role in connecting various major fields, such as chemistry, physics, engineering, and material science. They are used in these sectors based on their widespread applicability in optoelectronic devices, including organic light-emitting diodes [2], organic field-effect transistors [3, 4], sensors [5], organic photovoltaics [6], batteries [7], fuel cells [8, 9], and solar cells [10]. There have been numerous research studies on different types of CPs such as polypyrrole [11], polyaniline [12], polythiophene [13], poly(phenylenediamine) [14], poly(aminophenol) [15], and

poly(3,4-ethylenedioxythiophene) [16]. Oligofurans have been extensively investigated as oligothiophenes because the replacement of sulfur with oxygen reduces aromaticity and oxidation potential. Unlike thiophenes, furan-based materials are reportedly biodegradable and can be prepared from bio-renewable sources [17, 18]. Gidron et al. replaced thiophene with furan-based materials inside optoelectronic materials based on its high rigidity, strong fluorescence for optoelectronics, significant charge delocalization for charge transport in polymer films, desirable field-effect mobility for use in solar cells, and biodegradability [19]. The characterization and properties of poly(mono-, bi-, or trifuran) were investigated by Zhen et al. [20]. Research has shown that oligofurans exhibit higher fluorescence efficiency compared to oligothiophenes and oligoselenophenes. In 2014, Ninis et al. identified similarities between theoretical and experimental data on the electrochemical, electronic, and optical properties of polyfuran and its oligomers (nFu) [21]. A series of long chains of α -oligofuran containing three to nine rings exhibited significant π -conjugation. Additionally, their planarity makes them promising candidates for use in organic electronics because they can alter the properties of polymers. Therefore, researchers incorporated alkyl chains into polymers without distorting their planarity to

Joyanta K. Saha joys643@chem.jnu.ac.bd

Joonkyung Jang jkjang@pusan.ac.kr

¹ Department of Chemistry, Jagannath University, Dhaka 1100, Bangladesh

² Centre for Advanced Research in Sciences (CARS), Dhaka University, Dhaka 1000, Bangladesh

³ Department of Nanoenergy Engineering, Pusan National University, Busan 46241, Korea

improve solubility, stability, molecular packing, optical and photovoltaic properties, light-emitting applicability, concentration quenching, etc. [22]. Akkuratov et al. synthesized TBTBT (T, thiophene; B, benzothiadiazole) units with alkyl chains [23]. These side chains ameliorate solubility while increasing the band gap of the polymer and enhancing the photovoltaic performance of polymer units. Lombeck et al. increased both solubility and luminescence in a PCDTBT copolymer composed of alternating TBT and carbazole units through the addition of hexyl side chains at the TBT units [24]. They also balanced the solubility and planarity of PCDTBT materials with an increased number of side chains using thiophene rings. Hwang et al. synthesized quinoidal polymer, PQuBTV, with extended conjugation that exhibited high planarity [25]. Meanwhile, Jhang et al. developed highly planar semiconducting polymers P1-3 T and P2-3T2F. Their DFT calculations demonstrated that the fluorinated P2-3T2F polymer has more planar backbone conformation than non-fluorinated polymer P1-3 T [26]. Jin et al. synthesized the longest alkyl-substituted α -oligofuran [27]. The alkyl side chain negligibly affected the planarity of the polymer. Additionally, the resulting α -oligo(alkylfuran) was stable and highly fluorescent. Wood et al. illustrated that the aromaticity and noncovalent locks increase the planarity of polymer [28].

In this study, the impact of common gaseous analytes $(X=H_2O, CH_3OH, N_2H_4, H_2O_2, HCN, NH_3, SO_2, and CO_2)$ on the planarity of alkyl-substituted α -oligofurans (AOF) was investigated. The planarity of pristine 4AOF was compared to 4AOF in the presence of the analytes (4AOF-X). The change in the planarity of 4AOF in the presence of these gaseous molecules has been revealed through the study of interaction energy calculation, and natural bond orbital (NBO) analyses. The NCI-RDG approach was applied to provide an overview of the interaction types in the AOF-analyte complexes. The results of this study can contribute to the use of AOF in various fields of polymer science.

Computational methodology

The reference for the study was the optimized geometry of 4AOF with four furan rings, which was used to investigate interactions with different gaseous analytes. Eight considered gaseous analytes were H_2O , CH_3OH , N_2H_4 , H_2O_2 , HCN, NH₃, SO₂, and CO₂. All calculations presented herein were executed using the Gaussian 16 program [29]. Equilibrium structures along the reaction pathways were computed using the gradient-correlated density functional theory (DFT) with the M062X in combination with the allelectron 6-311G(d,p) basis set [30]. This functional is highly nonlocal functional with double the amount with nonlocal exchange. This is designed to be suitable for a combination of main-group thermochemistry, kinetics, and non-covalent interactions. In addition to the M06-2X method, we also evaluated the performance of gradient-correlated density functional theory (DFT) with the Becke three-parameter exchange function [31] and the Lee-Yang-Parr function [32] (B3LYP), which does not account for non-covalent interactions. Single point (SP) energies for all complexes were evaluated at MP2/6-311G(d,p) level [33]. To study the interactions between the analytes and 4AOF, the analytes were positioned 3.0 Å above the 4AOF, and optimization was performed at the aforementioned level of theory. The absence of a negative vibrational frequency confirmed the true minima for every 4AOF-X complex during vibrational frequency calculations. Optimized geometries were used at the same level of theory for all single-point calculations in the NCI-RDG analysis. NCI-RDG analysis was performed using a MULTIWFN 3.5 multifunctional wave analyzer [34]. The interaction energy of the 4AOF-X complexes was calculated using the following equation:

$$\Delta E_{int} = E_{4AOF-X} - E_{4AOF} - E_X \tag{1}$$

where E_{4AOF-X} is the total energy of the 4AOF-X complex, and E_{4AOF} and E_X are the total energies of pristine 4AOF and X, respectively. The interaction energy of all analyzed complexes was adjusted to account for the basis set superposition error (BSSE) [35].

Results

The 4AOF contains four furan rings. Rings 1 and 2, depicted in Fig. 1a, possess distinct chemical properties due to the substitution of a hydrogen atom with an alkyl chain in ring 1. Rings 1' and 2' exhibit the same characteristics as rings 1 and 2, respectively. The study of the impact of the analytes on the planarity of 4AOF was carried out by keeping them above rings 1 and 2. The planarity of 4AOF was analyzed using the modified Eq. (2) as described in the reference [36].

$$P = \frac{\sum_{i} \frac{||\theta_i| - 90|}{90}}{i}$$
(2)

Here, θ_i is the dihedral angle formed between two adjacent furan rings and ranges from -180° to 180° . Each bond between the two furan rings yields a value between 0 and 1, and the average value (P) also ranges from zero to one. If P equals 0, then the 4AOF is entirely out of the plane, thereby distorting its conjugated system. On the other hand, if P equals 1, the 4AOF is completely planar. Table 1 lists the P values for both pristine 4AOF and 4AOF-X complexes. The pristine 4AOF has a P value of 0.99. When analytes interact **Fig. 1** The optimized structures of 4AOF and 6AOF are shown in **a** and **b**, respectively. 4AOF contains four furan rings, while 6AOF contains six furan rings. The optimized structure of 4Fu, a polyfurane with four furan rings, is shown in **c**. The solid line in **a** represents the dihedral angle (P1), and the dashed lines represent the dihedral angles θ_l and θ_r . The atoms are represented as gray rings for carbon, red for oxygen, and white for hydrogen



on ring 2, the planarity of 4AOF remains unaltered except CH_3OH (0.94), and H_2O_2 (0.95). In these cases, two analytes (CH_3OH and H_2O_2) migrate over ring 1 during the interaction on ring 2. However, introducing analytes onto ring 1 of 4AOF, all analytes were found to result in distortion of the planarity (Figs. 2 and S1).

During the optimization of 4AOF-X geometries, the analytes shifted from the top of ring 1 to a position between the alkyl chain and ring 1 allowing for the interaction with both ring 1 and the alkyl chain. The impact of these interactions is discussed in the "NCI analysis" section. As shown in Table 1, the highest distortion of planarity occurred with the interaction of 4AOF and H₂O (0.88) (Fig. 2). To understand the cause of this distortion, the planarity between the alkyl chain and furan ring was analyzed by measuring the dihedral angles θ_l and θ_r of the leftand right-side alkyl chains, respectively. In the isolated 4AOF, the two dihedral angles were both equal to 179.99°, showing that the two alkyl chains were in the same plane as the furan chain. However, in 4AOF-H₂O, the two alkyl chains deviated from the plane with dihedral angles of θ_1 = 128.92 and $\theta_{\rm r}$ =116.22. When two chains deviate from their planes, the P value drops from 0.99 to a lower value (0.88), indicating a distortion of the planarity of 4AOF. Similarly, the *P*-values for CH₃OH, CO₂, H₂O₂ and SO₂ are lower than 0.99, with values of 0.91, 0.93, 0.94, and 0.94, respectively. This decrease in *P* value is due to the deviations of two alkyl chains from their plane when these analytes interact with ring 1, resulting in dihedral angles lower than 179.99 (as shown in Table 1). To further verify this observation, the effect of the analytes on the planarity of tetrafuran (4Fu), which lacks alkyl chains, was studied. Here, the chemical nature of every ring in 4Fu is the same. The two analytes H₂O and CH₃OH were maintained on ring 2 of 4Fu (Fig. 3). The P-value of 4Fu remains unchanged at 0.99 both before and after interacting with

4AOF-X	Ring 1			Ring 2		
	P	θ_l	θ_r	P	θ_l	θ_r
4AOF	0.99	179.99	179.99	0.99	179.99	179.99
4AOF-H ₂ O	0.88	128.92	116.22	0.99	179.88	179.86
4AOF-CH ₃ OH	0.91	124.63	70.08	0.94	167.46	117.84
4AOF-CO ₂	0.93	135.28	135.29	0.99	178.83	178.88
4AOF-H ₂ O ₂	0.94	126.19	78.77	0.95	126.11	78.63
4AOF-SO ₂	0.94	164.32	164.54	0.94	75.80	174.69
4AOF-N ₂ H ₄	0.97	174.31	171.31	0.99	179.80	179.69
4AOF-NH ₃	0.98	116.93	177.47	0.99	179.78	179.57
4AOF-HCN	0.99	179.36	167.90	0.99	179.51	179.88

Table 1 The planarity (P) of4AOF and dihedral angles θ_l and θ_r have been tabulated



Fig.2 The optimized geometries of 4AOF with four different analytes: a H_2O , b CH_3OH , c CO_2 , and d H_2O_2 . These analytes interacted on ring 1 of the 4AOF

the two analytes, indicating that its planarity is not altered. This is because 4Fu does not have any alkyl substituents for the analytes to interact with. The P-values of 4AOF were found to be 0.97, 0.98, and 0.99 after interaction with the other three analytes N₂H₄, NH₃, and HCN, respectively (Fig. S1). This suggests that these analytes have a lesser impact on the distortion of the planarity of 4AOF as compared to the other five analytes. As mentioned above, when the analytes interact with 4AOF on ring 2 except CH₃OH and H₂O₂, the P-values of 4AOF-X are 0.99. This is due to the two alkyl chains still being in the same plane as the furan chain, with θ_l and θ_r values close to 179° (Figs. 4 and S2). CH₃OH and H₂O₂ shift from ring 2 to ring 1 and approach the alkyl chains for interaction. To further explore this, 6AOF was studied where the analytes were allowed to interact with ring 3 (Figs. S3 and S4).



Fig. 4 Four analytes (**a** H_2O , **b** CH_3OH , **c** CO_2 , and **d** H_2O_2) interacting with ring 2 of 4AOF, where the planarity of 4AOF remains unaltered except CH_3OH and H_2O_2

The *P*-values for all analytes were found to be 0.99 in the case of 6AOF. This implies that the planarity of AOF is impacted when the analytes interact with ring 1 and can merge with an alkyl substituent. On the other hand, if the interaction occurs with rings that are far from ring 1 and lack an alkyl substituent, the planarity of AOF is maintained. It can be concluded that the planarity of AOF can be preserved when the analytes interact with rings distant from ring 1 with no alkyl substituent, but if they have the opportunity to interact with an alkyl substituent in ring 1, the planarity of AOF will be distorted.

The interaction energies (ΔE_{ad}) between 4AOF-X and the analytes were analyzed to determine the strength of interactions (Table 2). The results showed that when the analytes interacted on ring 1 of 4AOF, the ΔE_{ad} values were higher compared to ring 2. The maximum distortion of planarity was observed when H₂O interacted on ring 1, with ΔE_{ad}



Fig. 3 Optimized geometries of tetrafuran (4Fu) (a), tetrafuran with H_2O (b), and CH_3OH (c)

 Table 2
 The interaction energies of different analytes on rings 1 and

 2
 of 4AOF computed at M06-2X/6-311G(d,p) level of theory. All energy values have been corrected with BSSE

4AOF-X	ΔE (kcal/mol)			
	Ring 1	Ring 2		
4AOF-H ₂ O	-4.55 (-2.56) ^a	-2.90 (-1.63)		
4AOF-CH ₃ OH	-7.61 (-6.07)	-5.88 (-4.56)		
4AOF-CO ₂	-4.51 (-3.59)	-3.08 (-2.53)		
4AOF-H ₂ O ₂	-8.76 (-6.50)	-8.76 (-6.49)		
4AOF-SO ₂	-7.74(-5.78)	-6.48 (-6.04)		
4AOF-N ₂ H ₄	-7.71 (-6.21)	-7.44 (-5.71)		
4AOF-NH ₃	-4.82 (-3.13)	-2.60 (-1.68)		
4AOF-HCN	-4.53 (-3.81)	-4.24 (-3.53)		

^aThe values in parenthesis were corrected for zero-point vibrational energies (ZPE)

value of -4.55 kcal/mol. The other analytes also showed higher ΔE_{ad} values on ring 1 compared to ring 2, with values ranging from -8.76 kcal/mol to -4.53 kcal/mol. These results suggest that ring 1 of 4AOF has stronger interactions with the analytes compared to ring 2. Likewise, compared to ring 2, ring 1 of 4AOF exhibited stronger interaction energies with the analytes, as shown in Table S1 obtained at the B3LYP/6-311 g(d,p) level of theory. However, these interaction energy values are lower than those obtained from the M06-2X/6-311 g(d,p) level of theory, since M06-2X/6-311 g(d,p) is more adept at handling non-covalent interactions than B3LYP and other DFT functionals [37]. The interaction energies of all complexes calculated with MP2/6-311 g(d,p) level are shown in Table S1.

NBO analysis

To study the interactions between analytes and 4AOF on rings 1 and 2, the NBO analysis was conducted. This analysis evaluates the donor-acceptor interactions in a complex. E^2 is the second-order perturbation energy in a donor and acceptor interaction based on $n \to \sigma^*$ or $\sigma \to \sigma^*$ charge transfer. When H₂O interacts on rings 1 and 2 of 4AOF, the highest E^2 values of 3.06 and 0.51 kcal/mol are seen for $n_{O58(4AOF)} \rightarrow \sigma^*_{O67-H69(H_2O)}$ and $n_{O67(H_2O)} \rightarrow \sigma^*_{C59-H65(4AOF)}$ interactions, respectively. Here, 4AOF interacts with H₂O through H-bonds. The E^2 values indicate that H₂O interacts stronger with ring 1 than ring 2 of 4AOF. When CH₃OH interacts with ring 1, the highest stabilization energy E^2 value of 0.66 kcal/mol is seen for $\sigma_{C61-C62(4AOF)} \rightarrow$ $\sigma^*_{O71-H72(CH_3OH)}$ interaction. On ring 2, the maximum value is seen as 1.15 kcal/mol for $n_{O71(CH_3OH)} \rightarrow \sigma^*_{C23-H24(4AOF)}$. Here, CH₃OH acts as a donor. In the case of CO₂, the maximum E^2 value is observed when it interacts with 4AOF on ring 1 (0.79 kcal/mol for $\sigma_{C39-C40(4AOF)} \rightarrow \sigma^*_{C67-C68(CO_2)}$ interaction) than on ring 2 (0.51 kcal/mol for $\sigma_{C61-C62(4AOF)} \rightarrow \sigma_{C67-C68(CO_2)}^*$ interaction). The $\sigma_{C61-C62(4AOF)} \rightarrow \sigma_{O68-H69(H_2O_2)}^*$ interaction indicates the flow of charge transfer from 4AOF to H₂O₂ on rings 1 and 2. These interactions contribute 0.74 and 0.75 kcal/mol for stabilization. For N₂H₄, SO₂, NH₃, and HCN, the most effective interactions $\sigma_{N68-H71(N_2H_4)} \rightarrow \sigma_{C53-C54(4AOF)}^*$; $\sigma_{C53-C54(4AOF)} \rightarrow \sigma_{S67-O69(SO_2)}^*$; $\pi_{N67(NH_3)} \rightarrow \sigma_{C7-H9(4AOF)}^*$; $\sigma_{C61-C2(4AOF)} \rightarrow \sigma_{H68-C69(HCN)}^*$ are found on ring 1 with stabilization energies of 0.34, 1.67, 0.72, and 0.67 kcal/mol, respectively. The most effective interactions ($\pi_{N68(N_2H_4)} \rightarrow \sigma_{C53-C54(4AOF)}^*$; $\sigma_{C61-C2(4AOF)} \rightarrow \sigma_{S67-O69(SO_2)}^*$; ($\sigma_{N67-H70(NH_3)} \rightarrow \sigma_{C53-C54(4AOF)}^*$; $\sigma_{C61-C2(4AOF)} \rightarrow \sigma_{H67-C68(HCN)}^*$) on ring 2 are stabilized with energies of 0.54, 1.25, 0.25, and 1.54 kcal/mol, respectively. Ring 2 interactions are weaker except for HCN.

NCI analysis

The NCI-RDG approach was employed to determine the interaction types between 4AOF and analytes. This method enables the thorough identification and visualization of hydrogen bonds, van der Waals interactions, and steric effects. The 2D scatter map and 3D color-filled RDG isosurfaces of 4AOF are presented in Fig. 5. The isosurfaces were colored on a blue-green-red scale based on the values of sign(λ_2) ρ ranging from -0.035 to +0.02 a.u. The RDG (s) isosurface value is set to 0.65. In the NCI approach, large negative values of sign($\lambda 2$)*r* are represented by blue regions, indicating attractive interactions like dipole-dipole or hydrogen bonding. On the other hand, red regions with positive values signify nonbonding interactions and indicate steric hindrance. Sign $(\lambda_2)\rho \approx 0$ indicates a very weak van der Waals (vdW) interaction. In Fig. 5 (left), two disclike green-red isosurfaces are present between the hydrogen atoms of -C1H2 and the oxygen atom of furan ring 1, as well as between the hydrogen atoms of -C2H2 and the hydrogen atom of furan ring 1. These represent very weak van der Waals (vdW) interactions, as indicated by spikes at $sign(\lambda 2)\rho$ values -0.01 and +0.01 a.u. in the scatter map (Fig. 5, right).

These vdW interactions help to keep the alkyl chain aligned with the plane of the furan ring. Likewise, two disc-like green-red isosurfaces are visible for the rightside alkyl chain. The presence of steric interactions within each furan ring is shown by the red color of the related isosurfaces. When the analytes interact with 4AOF on ring 2, disc-like green-red isosurfaces appear between the two, representing very weak vdW interactions (Fig. S7). However, the vdW interactions between the alkyl chains, and rings 1 and 1' remain unchanged, preserving the planarity of like 4AOF. When the analytes interact with ring 1 of



Fig. 5 NCI isosurface (left) and NCI index plot (right) of 4AOF at "s"=0.65. Blue color indicates strong attractive interaction and red color indicates strong repulsive interaction



4AOF, the interaction affects both ring 1 and the alkyl chains, as indicated by the green-red disc isosurfaces between the analytes and alkyl chain/ring 1 (Figs. 6 and S6). The alkyl chains either protrude out of or lie within the horizontal plane of the furan ring. It is noteworthy that among the four green-disc isosurfaces that preserve the planarity of the isolated 4AOF (Fig. 5), one or two are missing in the complexes, leading to a destruction of the planarity of the alkyl chains and deflection.

Conclusion

Using DFT, we investigated the impact of various common gas molecule analytes on the planarity of AOF. Our results showed that gases could interact with either ring 1 or 2 of AOF. The maximum planarity distortion of 4AOF was observed for H₂O (P=0.88) on ring 1. However, the interaction with ring 2 did not alter the planarity. Similarly, stronger interaction values were observed for the interactions on ring 1 compared to ring 2. NBO and NCI analyses were conducted to compare the interactions between the analytes and the rings, revealing that the weak van der Waals interactions between the alkyl chains and furan ring contribute to maintaining planarity. However, when the analytes interact with ring 1, these interactions are disrupted, leading to planarity distortion. If gases interact with distant rings from the alkyl chains, AOF can maintain its planarity. This study highlights the influence of gaseous analytes on the planarity of AOF, which has implications for its various applications.

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Availability of data and materials Not applicable.

Declarations

Competing interests The authors declare no competing interests.

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