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X-ray crystallography and computational studies of the structure of bis-nitrone, 2,5-bis{[methyl(oxido)imino]phenyl}-furan

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1. Introduction

ABSTRACT

Bis-nitrone, 2,5-bis{[methyl(oxido)imino]phenyl}-furan prepared by condensation of 2,5-diformylfuran with two equivalents of phenylhydroxylamine can theoretically exist in 10 different structural isomeric forms. The relative energies calculated with AUG-cc-pVDZ and 6-311+G(df, pd) basis sets are used to predict the most stable isomeric form for this molecule. The single crystal X-ray structure analysis confirms this prediction. The bond lengths, angles, and dihedral angles obtained in the crystal structure are in good agreement with the molecular parameters calculated using DFT B3LYP method employing 6-311+G(df, pd) basis set. Population analysis using polar tensors (APT) indicates the traditional N⁺ $-O^-$ interpretation of the nitrone function whereas Mülliken method fails to show the charge separated structure.

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Nitrones are an attractive class of compounds due to their wide spectrum of applications as, 1,3-dipoles in organic synthesis [1], spin traps in free radical probes [2], polymer stabilizers [3], and metal chelating ligands [4]. These compounds are generally prepared by condensation of aldehydes with hydroxylamines or by oxidation of N-hydroxyl secondary amines. The geometries of these nitrones are important in their ability to form metal complexes, cycloaddition reactions, as well as to understand the hyperfine coupling in the EPR signals in spin trap applications [5]. Merino et al. has shown that, N-benzyl-C-(2-pyridyl) nitrone [6], and *N*-[(2*S*)-2-(*tert*-butoxycarbonylamino)propylidene] benzylamine N-oxide [7] exists in the Z-geometry, using X-ray crystallography. In contrary to this observation, C-alkoxy nitrones like C-ethoxy-C-phenyl-N-methylnitrone are known to exist as mixtures of *E* and *Z* isomers [8]. Due to the unique C=N–O moiety, nitrones are fascinating and challenging topics for computational chemistry as well. Compounds with two nitrone groups, bis-nitrones, are a rare class of compounds, and only a handful of bis-nitrones are reported in literature [9,10], and these include the recently reported, 6,6'-bis{methyl(oxido)imino]methyl}-2,2'-bipyridine [9], which form stable complexes with Cu(II), Ni(II), Co(II), and Cr(III) ions. Furthermore, the geometry of the free ligand is not reported in these studies. Our interest in the synthesis of 2,5-diformylfuran [11] as a renewable resources based feedstock chemical, and applications in the synthesis of polymeric materials [12] have led us to the preparation of the corresponding bis-nitrone, 2,5-bis{[methy-l(oxido)imino]phenyl}-furan. This symmetrical bis-nitrone can theoretically exist in 10 different isomeric forms (**1a–j**) as shown in Fig. 1. In this communication we will show the synthesis and characterization of bis-nitrone, demonstrate the application of computational methods for the prediction of the most stable isomeric form for this bis-nitrone, and compare the calculated bond distances and bond angles with the X-ray crystallography data.

2. Experimental

2.1. Materials and physical measurements

2,5-Diformylfuran was prepared using our previously published procedure [11]. *N*-Phenylhydroxylamine was freshly prepared by Zn—NH₄Cl reduction of nitrobenzene [13]. ¹H NMR spectra were recorded in CDCl₃ on a Varian Mercury plus spectrometer operating at 400 MHz and chemical shifts are given in ppm downfield from TMS (δ = 0.00). ¹³C NMR spectra in CDCl₃ were recorded in the same spectrometer operating at 100 MHz; chemical shifts were measured relative to CDCl₃ and converted to δ (TMS) using δ (CDCl₃) = 77.00. FT-IR spectra were recorded on a JASCO-470 PLUS IR spectrometer using KBr pellets. Elemental analysis was performed at QTI laboratories, New Jersey.





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Fig. 1. Possible isomeric structures of 2,5-bis{[methyl(oxido)imino]phenyl}-furan (1).

2.2. Synthesis of 2,5-bis{[methyl(oxido)imino]phenyl}-furan (1)

A mixture of 2,5-diformylfuran [11] (0.186 g, 1.5 mmol) and *N*-phenylhydroxylamine (0.327 mg, 3.0 mmol) in 10 mL of ethanol was heated at 50 °C for 15 min. Then the solution was allowed to stand at room temperature for 24 h, to give 2,5-bis{[methyl(oxido)imino]phenyl}-furan. The product was recrystallized from ethanol to give pale yellow crystals, 0.381 g, 83% yield, m.p. 194–96 °C. Found: C, 70.35; H, 4.83; N, 8.90%. Calc. for $C_{18}H_{14}N_2O_3$: C, 70.32; H, 4.61; N, 9.15%.

IR (KBr) 653, 684, 763, 819, 868, 1013, 1076, 1162, 1379, 1481, 1543, 3031, 3158 $\rm cm^{-1}.$

¹H NMR δ 7.47–7.53 (m, 6H), 7.79–7.82 (m, 4H), 8.16 (s, 2H), 8.17 (s, 2H).

¹³C NMR δ 119.0, 121.3, 123.6, 129.5, 130.6, 147.6, 148.8.

2.3. Theoretical calculations

All of the theoretical studies used density functional theory (DFT) in Gaussian 03 package [14]. Geometry optimizations were carried out with Becke hybrid exchange functional and the Lee–Yang–Parr correlation function (B3LYP) [15] using Pople-style basis sets (6-311+G(df, pd)) including diffuse (denoted by "+" for Pople-style). Single point energy calculation was carried out using AUG-cc-pVDZ. Frequency calculations were performed for all structures, and this vibrational frequency analysis yielded no imaginary frequencies.

2.4. X-ray diffraction data

The single crystals suitable for X-ray crystallography were grown by dissolving the 2,5-bis{[methyl(oxido)imino]phenyl}-furan (1) in methylenechloride, layering with pentane, and allowing the undisturbed solution to stand at room temperature for three days. X-ray crystallography data were collected on a Bruker SMART APEX II CCD diffractometer (Mo K\alpha-radiation, graphite monochromator, ω and φ scan modes) and corrected for absorption using SADABS program [16]. Crystals of 1, C_{18.5}H₁₅ClN₂O₃, M = 348.77, are monoclinic, space group $P2_1/c$, at 100 K: a = 15.632(2), b = 9.9648(14), c = 10.4743(15) Å, $\beta = 98.268(2)^{\circ}, V = 1614.7(4)$ Å³, Z = 4, $d_{\text{calc}} = 1.435 \text{ g cm}^{-3}$, $\mu(\text{Mo K}\alpha) = 0.257 \text{ mm}^{-1}$, $F(0\ 0\ 0) = 724$, λ (Mo K α) = 0.71073 Å, ω -scans 2 θ < 58°, number of reflections collected = 16,639. The structure was solved by direct methods and refined by full-matrix least squares technique with anisotropic displacement parameters for non-hydrogen atoms. The crystal of 1 contains a dichloromethane solvent molecule disordering over two sites related by the inversion center. The hydrogen atoms were placed in calculated positions and refined in riding model with fixed displacement parameters $(U_{iso}(H) = 1.2U_{eq}(C))$. All calculations were carried out by using the *SHELXTL* program [17]. Crystallographic data for **1** have been deposited with the Cambridge Crystallographic Data Center with deposition number CCDC 732,241. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033).

3. Results and discussion

3.1. IR and NMR spectroscopy

Bis-nitrone, 2,5-bis{[methyl(oxido)imino]phenyl}-furan (1) was prepared by condensation of 2,5-diformylfuran with two equivalents of N-phenylhydroxylamine, and was characterized by elemental analysis, IR and NMR spectroscopy. The IR spectrum of 1 shows a strong peak at 1076 cm⁻¹ indicating the N–O absorptions of the nitrone functions. The furan ring is indicated by the peaks at 653 and 684 cm⁻¹ Proton NMR spectrum of this compound shows two singlets at 8.16 (s, 2H) and 8.17 (s, 2H) ppm corresponds to furan ring protons and the --CH=-N- protons of the nitrone groups. The two multiplets, 7.47-7.53 (m, 6H), 7.79-7.82 (m, 4H) represents the phenyl groups of the compound. The ¹³C NMR spectrum shows seven signals confirming the symmetrical nature of the structure. The signals at 147.6 and 119.0 ppm can be assigned to furan ring carbons C-2 and C-3, respectively, whereas the phenyl ring carbons are observed at 121.3, 123.6, 129.5 and 130.6 ppm. The two nitrone carbons are assigned to the signal at 148.8 ppm.

3.2. Theoretical calculations

Structural studies on bis-nitrone **1** enables us to explore the geometric and electronic structure of a molecule with two conjugated nitrone moieties, as this compound can exist in 10 possible isomeric forms as shown in Fig. 1. The relative energies calculated for these isomeric structures (**1a**–**j**) using AUG-cc-pVDZ and 6-311+G(df, pd) basis sets and the relative energies with zero-point energy correction (ΔE_{ZPE}°), enthalpy (ΔH°) and free energies (ΔG°) corrected to room temperature are shown in Table 1.

Out of the 10 isomeric structures studied, the lowest energy conformation is from the structure **1b** as shown in Table 1. This minimized geometry of **1b** showed a small curvature in the structure and flat form of this geometry (**1b-flat**) showed a slightly higher values except in $\Delta E_{\text{ZPE}}^{\circ} @ 6-311+G(df, pd)$ calculation. However, the energy difference between **1b** and its flat form **1b-flat** is minimal, which suggests the geometry curvature impact on the π -delocalization system is minimal. The next two possible candidates are **1i** and **1j** isomeric structures, which only differs by the placement of phenyl group and O atom relative to the C=N bond.

Table 1
The relative energies of $1a-i$ calculated using AUG-cc-pVDZ and 6-311+G(df, pd) basis sets (kcal/mol).

Isomeric structure	ΔE° @ AUG-cc-pVDZ	$\Delta E^{\circ} @ 6-311+G(df, pd)$	$\Delta E_{\text{ZPE}}^{\circ}$ @ 6-311+G(df, pd)	$\Delta H^{\circ} @ 6-311+G(df, pd)$	$\Delta G^{\circ}@$ 6-311+G(df, pd)
1a	15.85	17.50	17.07	17.24	16.79
1b	0.00	0.00	0.00	0.00	0.00
1b-flat	1.17	0.91	-0.11	3.38	0.55
1c	12.76	14.05	13.46	12.57	14.98
1d	12.77	14.05	13.47	12.58	14.95
1e	16.89	17.51	17.13	16.14	18.97
1f	15.96	17.18	16.73	16.88	16.13
1g	12.62	13.85	13.52	13.66	12.88
1h	15.96	17.18	16.73	16.88	16.13
1i	7.71	8.11	7.87	7.93	7.55
1j	4.80	5.86	5.50	4.52	7.38

Examining the arrangements at the C=N bonds relative to the furan ring, one can see that isomeric structures **1a**-**d** have higher symmetry compared to the structures **1e**-**j**. However, structures **1a**, and **1d** have both nitrone moieties in the *E*-configuration. Additionally these two phenyl groups of **1d** will actually overlap each other in order to maintain a higher symmetry. Thus, the final optimized geometry has to lower its symmetry and even lose its Cs symmetry. The isomeric structure **1c** has the negatively charged oxygen atoms in close proximity, making it another high energy structure. Separate frequency calculations were carried out using the same method and no negative frequencies were found in the lowest energy conformation **1b**, which further confirms its global energy minimum geometry. Though the **1b-flat** shows two low imaginary frequencies, both of these disappeared once a tighter convergence criterion is used. In order to give a better insight into the nature of the N–O bonds in the system, a population analysis using atomic polar tensors (APT) [18] was carried out for the symmetric structures **1a–d**. The popular atomic charge representation in common use is Mülliken population analysis. However, there are serious problems with this method due to the fact that this approach is based on projecting the electron density onto some reference basis set, which is related to the atomic orbital basis set. Here we will present the population analysis for structures **1a–d**, using APT (Table 2), which is not required to have direct reference to the basis set, and is readily available in the Gaussian output. Furthermore, Mülliken population analysis data for **1a–d** are also presented in Table 2, for comparison with the APT results. Table 2 clearly shows the failure of Mülliken interpretation of the N–O bond, which assigned negative charges to both N and O atoms. The APT population analysis

Table 2

The popu	ation analysis between N	—O using atomic	polar tensors (A)	PT) and t	raditional Mülliken	DOD	ulation anal	vsis fo	r isomeric	structures	1a-d	and	PBN.
	.	0											

	Mülliken population analysis					APT populati	on analysis			
	1a	1b	1c	1d	PBN	1a	1b	1c	1d	PBN
01 N1	-0.246 -0.118	-0.259 -0.193	-0.161 -0.195	-0.161 -0.195	$-0.374 \\ -0.094$	-0.112 0.935	-0.047 0.166	-0.030 0.012	-0.029 0.011	-0.622 0.287
С	-0.270	0.279	0.302	0.302	0.346	-0.0005	0.169	0.080	0.080	-0.014



Fig. 2. Front and side views of the single crystal X-ray structure of **1**, representation of atoms by thermal ellipsoids (*p* = 50%). Dichloromethane solvent molecule is omitted for clarity.



Fig. 3. The LUMO, HOMO, HOMO-1 and HOMO-2 orbital plot of 1b.

Table 3

The experimental and calculated bond lengths (Å), bond angles (°), and dihedral angles (°) in **1b** using DFT B3LYP method with 6-311+G(df, pd) basis set.

	Experime	ntal	Average	Calculated	Difference
Bond distance (Å)					
01–C2	1.377	1.376	1.3765	1.3702	0.006
C2-C3	1.373	1.377	1.3750	1.3821	-0.007
C3–C4	1.414		1.4140	1.4074	0.007
C2-C6	1.424	1.417	1.4205	1.4132	0.007
C6-N1	1.318	1.317	1.3175	1.3242	-0.007
N1-03	1.300	1.293	1.2965	1.2741	0.022
N1-C7	1.450	1.453	1.4515	1.4528	-0.001
С7—С8	1.392	1.387	1.3895	1.3907	-0.001
C8–C9	1.390	1.387	1.3885	1.3877	0.001
C9–C10	1.391	1.383	1.3870	1.3918	-0.005
C10-C11	1.384	1.387	1.3855	1.3908	-0.005
C11–C12	1.391	1.390	1.3905	1.3896	0.001
C12–C7	1.387	1.388	1.3875	1.3923	-0.005
Bond angle (°)					
C(2) - O(1) - C(5)	106.7		106.7	107.2	-0.500
O(3) - N(1) - C(6)	122.5	122.3	122.4	123.1	-0.700
N(1)-C(6)-C(2)	122.2	121.8	122.0	122.67	-0.670
O(3)-N(1)-C(7)	116.7	116.9	116.8	116.7	0.100
Dihedral angle (°)					
C3-C2-C6-N1	1.32	8.02	4.67	0.21	4.460
C2-C6-N1-C7	4.47	1.27	2.87	1.32	1.550
C6-N1-C7-C8	30.55	28.92	29.735	30.72	-0.985
C7–C8–C9–C10	0.88	0.89	0.885	0.4	0.485

assigns negative charges for the O atoms, and positive charges for N atoms for all four isomers studied, and clearly conform to the typical organic chemistry interpretation of N⁺—O⁻ moiety. Nitrone group charge densities of the common spin-trap α -phenyl-*N*-tert-butylnitrone (PBN) in the *Z*-geometry were also calculated using the same method for comparison, and these results are shown in Table 2 as well. Mülliken population analysis of PBN showed negative charges for both N and O, whereas the APT results showed the correct charges for these atoms, again showing the inadequacy of the Mülliken analysis in the case of nitrone function. Additionally, we have studied the molecular orbital picture of the most stable isomer (**1b**) to further comprehend the electronic nature of the N—O bond, and Fig. 3 shows the lowest unoccupied molecular orbital (LUMO), highest occupied molecular orbital (HOMO), and two orbitals (HOMO-1 and HOMO-2) below HOMO.

It is interesting to point out that, while both HOMO and LUMO orbitals of **1b** are π -bond in character, the N1–O3 bond shows a strong anti-bonding character. However, the polarized N–O bond is better illustrated with HOMO-1 and HOMO-2, particularly, the HOMO-2 shows the second lone pair on the oxygen strongly polarized into the N \rightarrow O direction (Fig. 3). The electronic structure of σ bond between N–O (not shown) shows even larger electron density polarization over the oxygen atoms. These results suggest that the nitrogen atom possesses some hypervalent character in addition to the charge separated N–O bond proposed in the APT population analysis. This extra electron density over oxygen atom

suggests a good chelating site for the ligand to bind with metal ions.

3.3. Crystal structure

The ΔE° , ($\Delta E^{\circ}_{\text{ZPE}}$), ΔH° , and ΔG° calculations clearly shows **1b** as the most favored structural isomer and this is consistent with the single crystal structure, as shown in the Fig. 2. The bond lengths, bond, and dihedral angles in the structure **1b** were calculated using DFT B3LYP method with 6-311+G(df, pd) basis set and a comparison of these calculated parameters with the experimental results obtained in the crystallographic analysis are shown in the Table 3. The calculated bond lengths of structure 1b are in excellent agreement with the experimental results in comparison to the bond angles. The differences in bond lengths are less than 0.022 Å, whereas the discrepancy in the bond angles is 0.7°. The largest discrepancy lies in dihedral angles, and is clearly shown in the dihedral angel of C3-C2-C6-N1, which has an average value of 4.67° in the crvstal structure, whereas the calculated value is 0.21°. The C2-C6 bond, which is the link between the furan and C=N moiety is 1.4205 Å, while the C=N bond in the nitrone group has an average length of 1.3175 Å, and both these values are in excellent agreement with the calculated values. The calculated N1-O3 bond length, 1.2741 Å is slightly lower than the experimentally observed average N–O bond distance, which is 1.2965 Å. Both the calculated and experimental bond lengths are much longer than the mean value for the N–O bond in nitrates, as reported in the Cambridge structural database [19], which is 1.231 ± 0.025 Å. However, the calculated and experimental average N-O bond lengths of 1b are much closer to the experimental gas-phase value for N-O bond length in pyridine N-oxides (1.29 Å) [20]. The zwitterionic N⁺-O⁻ form is widely used to represent the N-O bond in nitrone and N-oxide compounds, nevertheless biradical and hypervalent canonic forms are also suggested for nitrone compounds [21].

4. Conclusion

In conclusion, we have correctly predicted the most energetically favored isomeric structure of 2,5-bis{[methyl(oxido)imino]-phenyl}-furan and shown that molecular parameters calculated using DFT B3LYP method with 6-311+G(df, pd) basis set are in good agreement with crystallographic data of the compound. Population analysis of the most favored isomeric structure using polar tensors (APT) indicates the traditional N⁺ $-O^-$ interpretation of the nitrone function whereas the molecular orbital plot indicates some hypervalent character in the nitrone nitrogen.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.molstruc.2010.05.029.

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