ORIGINAL PAPER

X-Ray Diffraction and Theoretical Approach to the Molecular Structure of (E)-2-(2-(1,3-dioxoisoindolin-2-yl)-1-(3-phenyl-3methylcyclobutyl)ethylidene) hydrazine carboxamide

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Abstract The title molecule (I), (E)-2-(2-(1,3-dioxoisoindolin-2-yl)-1-(3-phenyl-3-methylcyclobutyl) ethylidene) hydrazine carboxamide ($C_{22}H_{22}N_4O_3$), was synthesized and characterized by IR spectroscopy and single-cyrstal X-ray diffraction. The compound cyrstallizes in the triclinic space group P-1. In addition, the molecular geometry, vibrational frequencies and frontier molecular orbitals analysis of the title compound in the ground state have been calculated by using the HF/6-31G(d) and B3LYP/6-31G(d) methods. Molecular electrostatic potential of the compound was also performed by the theoretical method.

Keywords X-ray structure determination \cdot DFT and HF calculation \cdot B3LYP \cdot IR spectrum

Introduction

Isoindolinones and their derivatives have been investigated widely due to their profound physiological and

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A. Cukurovali Department of Chemistry, Faculty of Science, Firat University, 23119 Elazig, Turkey chemotherapeutic properties. Many compounds containing the isoindolinone skeleton have shown antiviral, antileukemic, antiinflammatory, antipsychotic and antiulcer properties [1, 2]. Isoindolinones are useful for the synthesis of various drugs and naturally occurring compounds [3, 4]. At the same time, it has been found that some isoindole-1,3-dione derivates have protein kinase CK2 (Casein Kinase) activity [5]. It is also well known that Phthalimides and N-substituted phthalimides are an important class of compounds because of their interesting biological activities [6]. Phthalimides have also served as starting materials and intermediates for the syntheses of alkaloids [7] and pharmacophores [8]. In addition, these compounds containing cyclobutane and phthalimide functions appear to be suitable candidates for further chemical modifications and may be pharmacologically active and useful ligands in coordination chemistry [9].

In this study, we report the characterization of (I) by using single crystal X-ray. In addition we also have determined the molecular geometry, vibrational spectra, and frontier molecular orbital properties of this compound by using density functional theory (DFT) the Hartree–Fock (HF) [10], density functional using Becke's three-parameter hybrid functional [11] with the Lee, Yang, and Parr correlation functional methods (B3LYP) [12]. Therefore, we compare theoretical calculations and X-ray experimental data.

Results and Discussion

X-Ray Crystallography

The data collection was performed at 293 K on a Stoe-IPDS-2 diffractometer equipped with a graphite monochromated Mo K α radiation ($\lambda = 0.71073$ Å) [13]. The structure was solved

Table 1 Crystallographic data for compound (I)

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Formula	$C_{22}H_{22}N_4O_3$
Molecular weight	390.44
Temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions (Å, °)	
a	5.7444(4)
b	11.7325(8)
С	15.6240(12)
α	76.688(6)
β	85.672(6)
γ	79.995(6)
Volume	1008.43(13)
Ζ	2
Calculated density (g cm ⁻³)	1.286
T_{\min}, T_{\max}	0.9595, 0.9974
$\mu (\mathrm{mm}^{-1})$	0.09
θ_{\max} (°)	26.5
Index ranges	$h = -7 \rightarrow 6, k = -14 \rightarrow 14$ $l = -19 \rightarrow 19$
Reflections collected	8,686
Independent reflections	4.141
Observed reflections $(I > 2\sigma)$	1.684
S	0.94
$R (I > 2\sigma)$	0.065
$wR \ (I > 2\sigma)$	0.113
$S = R \ (I > 2\sigma)$ $wR \ (I > 2\sigma)$	0.94 0.065 0.113

direct methods using SHELXS-97 [14], and refined by a fullmatrix least-squares procedure using the program SHELXL-97 [15], molecular graphics ORTEP-3 for Windows [16]. All







Fig. 1 The molecule of compound $\left(I\right)$ showing the atom labelling scheme

hydrogen atoms were included using a riding model and refined isotropically with C–H = 0.93–0.97 Å and N–H = 0.86 Å. $U_{iso}(H) = 1.2U_{eq}$ (C, N), $U_{iso}(H) = 1.5U_{eq}$ (for methyl group). Details of the data collection, cyrstal parameters and refinements are given in Table 1.

Computational Method

DFT calculations are carried out with Gaussian 03 program [17]. B3LYP hybrid method which uses Becke's three parameter exchange functional gradient corrected functional. Lee et al. was used to predict the minimum energy molecular geometry of the title compound. The molecular structure of (I) in the ground state (in vacuo) was optimized by DFT(B3LYP) [18] with the 6-31G(d) [19] and HF



Table 2 Hydrogen bonding geometries for (I)

D–H…A	D-H(Å)	$H{\cdots}A(\mathring{A})$	$D{\cdots}A(\mathring{A})$	D-H···A(°)
N2–H2···O3 ⁱ	0.86	2.06	2.901(3)	167
C12–H12···O3 ⁱ	0.98	2.47	3.202(4)	132
C8–O2···Cg(2) ⁱⁱ	0.96	3.339(4)	3.869(6)	106.8(3)
Symmetry code:	(i) $-x + 1$,	-y + 1, -z	+ 1, (ii) 1 -	x, 1 - y, -z

 Table 3 Selected theoretical and experimental geometric parameters in the title compound

Parameters	Experimental	HF/ 6-31G(d)	B3LYP/ 6-31G(d)
Bond lengths (Å)			
O1–C1	1.215(6)	1.188	1.214
O2–C8	1.214(7)	1.188	1.214
O3-C11	1.225(4)	1.206	1.223
N1-N2	1.382(3)	1.360	1.363
N1-C10	1.272(4)	1.256	1.284
N2-C11	1.357(4)	1.378	1.400
N4-C1	1.383(6)	1.387	1.405
N4-C8	1.385(6)	1.386	1.404
C1-C2	1.487(7)	1.492	1.494
C2–C7	1.374(9)	1.381	1.397
C7–C8	1.471(8)	1.492	1.493
C12-C13	1.549(5)	1.554	1.567
C14-C15	1.552(5)	1.554	1.565
Bond angles (°)			
N2-N1-C10	117.7(2)	119.4	119.2
C1-N4-C9	123.3(3)	123.3	123.5
C1C2C7	108.5(5)	108.1	108.3
N2-C11-N3	116.4(3)	115.8	114.6
C8-N4-C9	124.1(4)	123.3	123.6
O1C1N4	125.0(4)	125.6	125.3
O3-C11-N3	122.5(3)	124.2	125.3
Torsion angles (°)			
C10-N1-N2-C11	170.2(3)	174.4	174.9
C2C1N4C9	-177.3(3)	172.4	173.7
C9-C10-N1-N2	-179.2	179.7	-179.9
N4-C9-C10-C12	176.8(3)	177.4	177.2
O1-C1-C2-C7	177.0(5)	179.5	-179.9
N1-C10-C12-C15	176.9(3)	176.7	177.7

methods. The ground state geometries were obtained in the gas phase by full geometry optimization, starting from the structural data.

Description of the Crystal Structure

The compound (I) crystallizes in the triclinic space group P-1 with two molecules in the unit cell. The crystal



Fig. 3 Atom-by-atom superimposition of the structures calculated (*red*) [a HF/6-31G(d), b B3LYP/6-31G(d)], on the X-ray structure (*black*) for the title compound. Hydrogen atoms have been omitted for clarity (Color figure online)

formula structure with the, C22H22N4O3, (I) shown in Fig. 1. The title molecule is composed of isoindolinone group, phenyl, semicarbazone and cyclobutane moieties. The molecule adopts E geometry about azomethine C=N double bond. The N2-N1=C10-C12 torsion angle being $-1.8(5)^{\circ}$ and N2–N1=C10–C9 torsion angle being -179.2° . In addition, the moiety of C10-N1-N2-C11-O3-N3 atoms is nearly planar, with a mean deviation of -0.085 Å for atom N1. The cyclobutane ring is puckered and the C13/ C14/C15 plane forms a dihedral angle of 18.6° with the C15/C12/C13 plane. This value is smaller than those, which literature values for the puckering of the cyclobutane ring are 26.8 (2)° [20], 23.5° [21] and 19.26 (17)° [22]. The isoindoline ring is nearly planar, with a mean deviation of 0.047 Å for atom N4. The two carbonyl, C1=O1 and C8=O2 bonds are almost same lengths with 1.214(6) Å and 1.213(7) Å, respectively. Similar value has been reported previously 1.204(3) Å [23]. Hydrogen bonding interactions of compound (I) will be seen in Fig. 2.

In the crystal packing, the molecules are linked to one another with N–H···O and C–H···O hydrogen bonding. In N–H···O hydrogen bonding, the atom N2 at (x, y, z) acts as a donor, via atom H2, to atom O3 at (-x + 1, -y + 1, -z + 1). Resulting in the formation of N–H···O mutual hydrogen bonds which link two molecules related by an



Fig. 5 The experimental FT-IR spectra of the title compound (1)

%

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inversion centre. This configuration is characterized by an $R_2^2(8)$ graph set [24]. $R_2^2(8)$ rings formed by hydrogen bonds are centred at (1/2 + n, 1/2 + m, 1/2) (*n*, *m*, are integer). On the other hand, atom C12 of cyclobutane ring behaves as a donor, via atom H12, to atom O3 in C–H···O intermolecular hydrogen bonds around inversion centres. Therefore, these hydrogen bonds generate bifurcated

hydrogen bonding. In addition, variations in O2=C8, C8–N4, N4–C1, C1–C2, C2=C7 and C7–C8 bond lengths (Table 3) confirm electron delocalization along the -O2=C8-N4-C1-C2=C7-C8- segment when compared with literature values for the isoindoline ring [23]. Then it can be said this electron delocalization may cause intermolecular interaction, namely, C8–O2…Cg(2) [Cg(2) is

 Table 4 Comparison of the observed and calculated vibrational spectra of the title compound

Assignments	Experimental (cm ⁻¹)	HF/6- 31G(d) (cm ^{-1})	B3LYP/6- 31G(d) (cm ⁻¹)
$v_{as}(NH_2)$	3535	3561	3581
$v_{\rm s}({\rm NH_2})$	3416	3445	3457
v(NH)	3186	3457	3431
v _s (CH) iso.	3087	3040	3098
v _s (CH) aromatic	2925	3024	3085
$v_{\rm s}({\rm CH_2})$	2858	2912	2948
$v_{\rm s}({\rm C=O})$	1768	1843	1738
$v_{as}(C=O)$	1714	1786	1737
v(C=O)	1693	1763	1760
v(C=N)	1550	1734	1645
β (NH)	1425	1463	1423
$\omega(CH_2) + \beta(CH)$	1251	1189	1217

Vibrational modes: v, stretching; β , bending; ω , wagging; s, symmetric; as, asymmetric; iso, isoindolinone ring



Fig. 6 Correlation graphics of calculated and experimental frequencies of the title compound. **a** HF and **b** DFT

N4/C1/C2/C7/C8]. The distance between O2 and the centroid Cg2 at (1 - x, 1 - y, -z) is 3.339(4) Å and C8–O2…Cg2 angle is 106.8(3)°. Beside of these, intramolecular N3–H…N1 hydrogen bond bring into existence S(5) graph set [24], details of these bonds and interaction are given in Table 2.

DFT and HF Calculations

The optimized structure parameters of the structure (I) calculated by DFT (B3LYP) and HF level with the 6-31G(d) basis set are listed in Table 3. As seen from Table 3, most of the optimized bond lengths are slightly longer than the experimental values and the bond angles are slightly different from the experimental ones. Because, the molecular states are different during experimental and theoretical processes. One isolated molecule is considered in gas phase in theoretical calculation, whereas many packed molecules are treated in solid phase during the experimental measurement. When the X-ray structure of (I) is compared with HF/6-31G(d) and B3LYP/6-31G(d) optimized counterpart (see Fig. 3), it can be easily seen that they are slightly different each other. The RMS fit of the atomic position of (I) to those of its HF and B3LYP optimized counterparts are 0.3012 and 0.2766 Å, respectively. Consequently, the B3LYP method correlates well for the geometrical parameters when compared with HF.

Owing to our calculations, HF and B3LYP methods correlate well for the bond length comparison. The largest differences between experimental and calculated bond lengths about 0.0238 Å for HF and 0.04258 Å for B3LYP. The bond angles provided by HF method is the closest to the experimental values (see Table 3). The largest difference is about 1.797° in the case of HF method, while this difference is 2.828° for B3LYP method. The same trend was also observed in torsion angles. The largest differences are 4.673° and 4.937° for B3LYP and HF methods, respectively. Although there are some differences between the theoretical and the experimental values, the optimized structural parameters can well reproduce the experimental ones and they are basis for the discussions hereafter. The correlation between the experimental and calculated geometric parameters is given in Fig. 4.

Infrared Spectra

Harmonic vibrational frequencies of (I) were calculated by using B3LYP and HF method with 6-31G(d) basis set and the obtained frequencies were scaled by 0.9613 and 0.8929 [25], respectively. The FT-IR spectra of (I) is shown in Fig. 5. The formation of hydrogen bonds causes the significant low-wavelength shift and broadening of N–H stretching mode, and it can be observed around 2500–3500 cm⁻¹ with multiple peaks [26]. In this study, the N2–H stretching mode is observed at 3186 cm⁻¹. On the other hand, N2–H bending mode is observed at 1425 cm⁻¹. This value is given with 1499 cm⁻¹ [27] in



0.0632 a.u.





Fig. 8 HOMO and LUMO of the title compound

the literature. As can be seen in Table 4 due to N2–H2…O3 intermolecular hydrogen bonding, experimental v(N-H) bending vibration increases while v(N-H) stretching vibration decreases [28]. The strong and broad band centered between 3096 and 2922 cm⁻¹ are attributed to asymmetric and symmetric C–H stretching vibrations of aromatic and aliphatic groups. v(C=O) vibrations are observed at 1771, 1726 and 1677 cm⁻¹ in the infrared experimental spectra, while the calculated values are 1843, 1786 and 1763 cm⁻¹ for HF, 1783, 1737 and 1760 cm⁻¹ for B3LYP, respectively. This difference given for C=O

stretching vibration can be explained by the existence of the C12–H12…O3 intermolecular hydrogen bond given in Table 2, because isolated molecules are taken into consideration in calculations [29]. Experimental frequencies of (I) were compared with calculated vibrational frequencies by correlation graphics given in Fig. 6. The correlation graphics in Fig. 6 show that experimental fundamentals are found to have a good correlation with calculations by B3LYP method when compared to HF method.

Molecular Electrostatic Potential

Molecular electrostatic potential maps provide the isosurface values with the location of negative and positive electrostatic potentials. The differences between nucleophilicity and electrophilicity may affect its the proton donating or accepting ability of the compound [30]. While the negative electrostatic potential corresponds to an attraction of the proton by the concentrated electron density in the molecule (and is colored in shades of red on the EPS surface), the positive electrostatic potential corresponds to repulsion of the proton by atomic nuclei in regions where low electron density exists and the nuclear charge is incompletely shielded (and is colored in shades of blue) [31].

Figure 7 shows the molecular electrostatic potential (MEP), was determined using B3LYP/6-31G(d) method. The different values of the electrostatic potential at the surface are represented by different colors. As can be seen in Fig. 7, the negative (red) region is localized on the unprotonated atom of, O3, with a minimum value of -0.0632 a.u. However, maximum positive (blue) region is localized on atoms C12 and N2 probably due to the hydrogen, with a maximum value of 0.0632 a.u. and green represents regions of zero potential. Therefore, Fig. 7 confirms the



Scheme 1 Synthesis scheme of the title compound (I)

existence of an intermolecular N–H…O and C–H…O interactions. In addition, the weak red regions associated with O1 and O2 atoms with a value of -0.043 a.u. And also the carbonyl oxygen atom, O2, is involved in intermolecular C8–O2…Cg(2) interaction. Therefore it can be said these sites give the information about the region from where the compound can have intermolecular interactions.

Frontier Molecular Orbitals Analysis

Figure 8 shows the distributions and energy levels of HOMO and LUMO orbitals of (I) by obtained at the B3LYP/ 6-31G(d) method. The calculations indicate that the title compound has 103 occupied molecular orbitals. While highest occupied molecular orbitals (HOMOs) localized on the semicarbazone moiety, lowest unoccupied molecular orbitals (LUMOs) are localized on the isoindoline ring. Because of that HOMO and LUMO are mainly localized on different parts of the title molecule, they are mostly the π -antibonding type orbitals. The value of the energy seperation between the HOMO and LUMO is 3.973 eV.

Experimental

Synthesis of the Title Compound

To a solution of phthalimide (1.4713 g, 10 mmol) in 50 mL ethanol, 1-methyl-1-phenyl-3-(2-chloro-1-oxoethyl) of cyclobutane (2.2271 g, 10 mmol) in 20 mL of absolute ethanol was added dropwise. End of the reaction was determined by monitoring the course of the reaction with IR spectroscopy. Subsequently, a solution of thiosemicarbazide (0.9113 g, 10 mmol) in 20 mL of absolute ethanol was added. After addition of thiosemicarbazide, the temperature was raised to 323-328 K and stirred at this temperature for 2 h. The solution was cooled to room temperature and then made alkaline with an aqueous solution of NH₃ (5%), and white precipitate separated by suction. washed with aqueous NH₃ solution several times and dried in air. Suitable single crystals for crystal structure determination were obtained by slow evaporation of its ethanol solution. Yield: 89%, melting point: 523 K. Characteristic IR bands: 35,345 and $3,416 \text{ cm}^{-1} v(-\text{NH}_2), 3,186 \text{ cm}^{-1} v(-\text{NH}_{-}), 2,967-2858$ 903

ν(aliphatics), 1768 and 1714 *ν*(C=O), 1693 (C=O), 1550 cm⁻¹*ν*(C=N). Characteristic ¹H NMR shifts (DMSOd₆, δ, ppm): 1.49 (s, 3H, -CH₃ on cyclobutane), 2.31–2.52 (m, 4H, -CH₂-, in cyclobutane ring), 3.84 (quint, *j* = 7.8 Hz, 1H, >CH- in cyclobutane ring), 4.38 (s, 2H, -CH₂-N), 5.77 (brs, 2H, -NH₂), 7.12–7.21 (m, 3H, aromatics), 7.26–7.37 (m, 2H, aromatics), 7.80–7.96 (m, 4H, aromatics), 9.26 (s, 1H, -NH). Characteristic ¹³C NMR shifts (DMSO-d₆, δ, ppm): 169.35, 158.45, 153.30, 147.83, 136.39, 133.33, 130.04, 127.18, 126.15, 124.93, 41.21, 38.62, 33.82, 31.02, 29.26 (Scheme 1).

Conclusions

(E)-2-(2-(1,3-dioxoisoindolin-2-yl)-1-(3-phenyl-3-methyl cyclobutyl)ethylidene) hydrazine carboxamide has been synthesized and characterized by IR and X-ray singlecrystal diffraction. The X-ray structure is found to be very slightly different from its optimized counterparts and the crystal structure is stabilized by N-H-O and C-H-O type hydrogen bonds. The theoretical calculations performed by HF and DFT (B3LYP) support the solid state structure. According to observed results, B3LYP method shows a better fit to experimental values than HF in evaluating geometrical parameters. It is noted here that the experimental results are for the solid phase and the theoretical calculations are for the gaseous phase. In the solid state, the existence of the crystal field together with the intermolecular interactions holds the molecules together, which results in differences between the calculated and experimental values for the bond parameters. The MEP map shows that the negative potential sites are on oxygen atoms as well as the positive potential sites are around the hydrogen atoms and so MEP map confirms the existence of intermolecular N-H···O and C-H...O interactions. Therefore, all the calculated spectra, bond lengths and angles of this structure are in good agreement with the experimental data.

Supplementary Material

Crystallographic data for the structure analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No 838406 Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: http://www.cede. cam.ac.uk).

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