Research Article

Crystal Structure, Spectroscopy, SEM Analysis, and Computational Studies of *N*-(1,3-Dioxoisindolin-2yl)benzamide

Hakan Bülbül,¹ Yavuz Köysal,² Necmi Dege,¹ Sümeyye Gümüş,³ and Erbil Ağar³

¹Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

²Yeşilyurt Demir Çelik Vocational School, Ondokuz Mayıs University, 55300 Samsun, Turkey

³Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

Correspondence should be addressed to Hakan Bülbül; hbulbul@omu.edu.tr

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The compound *N*-(1,3-dioxoisindolin-2yl)benzamide, $C_{15}H_{10}N_2O_3$, was prepared by the heating of an ethanolic solution of 2-hydroxy-1*H*-isindole-1,3(2*H*)-dione and 4-chloroaniline. The product was characterised using a combination of IR spectroscopy, SEM, and single crystal X-ray diffraction techniques. In addition to the experimental analysis, theoretical calculations were used to investigate the crystal structure in order to compare experimental and theoretical values. The X-ray diffraction analysis shows that the compound crystallises in the monoclinic space group $P2_1/c$ with the geometric parameters of $a = 13.5324(11)$ Å, $b = 9.8982(8)$ Å, $c = 9.7080(8)$ Å, and $\beta = 95.425(6)^\circ$. The crystal structure is held together by a network of $N-H \cdots O$ hydrogen bonds involving the carboxamide group.

1. Introduction

The molecular structure of *N*-(1,3-dioxoisindolin-2yl)benzamide contains isoindoline and benzamide moieties. Benzamide groups show various pharmaceutical activities including antiemetic, antipsychotic, and antiarrhythmic [1], anti-inflammatory, immunomodulatory, antitumoral, and antiallergic activities [2] and are also known to have important bioactive frameworks [3]. Isoindoline derivatives show anti-inflammatory, antipsychotic, antileukemic, antiviral, and antiulcer properties [4–6]. It is reported that disubstituted isoindolines display antibacterial, diuretic, and antitumor activity. Isoindolines, substituted with carboxylic acid groups, have been employed in SAR studies and also as candidates for organic light emitting diodes [7]. As a part of our ongoing research on benzamide and isoindoline derivatives, the title compound was synthesized and characterized by various methods.

2. Experimental

2.1. Synthesis and Crystallization. The compound *N*-(1,3-dioxoisindolin-2yl)benzamide (Scheme 1) was prepared by a refluxing mixture of a solution containing 2-hydroxy-1*H*-isindole-1,3(2*H*)-dione (0.0095 g 0.058 mmol) in 20 mL ethanol and a solution containing 4-chloroaniline (0.0158 g 0.116 mmol) in 20 mL ethanol. The reaction mixture was stirred for 1 h under reflux. The crystals of *N*-(1,3-dioxoisindolin-2yl) benzamide suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield 53%; m.p = 471–479 K).

2.2. Refinement. Data collection of the title compound, $C_{15}H_{10}N_2O_3$, was performed with STOE IPDS II single crystal X-ray diffractometer using graphite monochromated $MoK\alpha$ radiation ($\lambda = 0.71073$ Å) at room temperature (293 K). Cell parameters were obtained by using X-Area [8] and data reduction was achieved with X-RED32 [8] software.

FIGURE 1: Asymmetric unit of $C_{15}H_{10}N_2O_3$ (50% probability displacement ellipsoids).

SCHEME 1: Chemical diagram of title compound.

In total, 12087 reflections were collected with angles in the range $2.55^\circ < \theta < 27.66^\circ$ using the ω scan mode. The structure was solved and refined with SHELXS97 [9] and SHELXL-97 [9] software. Molecular graphics were created using ORTEP-3 [10]. WinGX [11] was used to prepare the data for publication.

All nonhydrogen atoms were refined anisotropically. The carboxamide hydrogen atom (H2A), bonded to (N2), was located in the Fourier difference map and refined isotropically. All other H atoms were placed geometrically and refined with their parent atoms with usable riding model [C-H = 0.93 Å for aromatic ring, $U_{iso}(H) = 1.2 U_{eq}(C)$]. The details of the experimental and refinement process are shown in Table 1.

3. Results and Discussion

3.1. Crystal Structure Description. The location the hydrogen atom on the N2 atom confirms that the structure adopts the amide form rather than the enolic form (Figure 1). The amide links the dioxoisindolin and arene groups. The individual aromatic rings in structure are essentially planar. The fused isoindoline ring is perfectly planar with a maximum deviation of 0.018(2) Å for C8, while the arene ring (C10–C15) is also planar with a maximum deviation of −0.007(4) Å for C13. The fused isoindoline ring makes a dihedral angle of 65.45 (7)° to the arene ring. The bond parameters in the structure are closely related to values in closely related structures [12–14]. The torsion angle C10–C9–N2–N1 is 179.68(18)° which confirms that the side chain conformation of the molecule is defined as the anticonformation. The independent molecules within the crystal are linked by N–H...O hydrogen bonds [N2–H2A...O3 with symmetry code (i): $x, -y + 1/2, z + 1/2$] that generate C4 motif [15] which links the molecules infinite

TABLE 1: Experimental details of $C_{15}H_{10}N_2O_3$.

Crystal data	
Empirical formula	$C_{15}H_{10}N_2O_3$
Formula weight	266.25
Colour, habit	Colorless, plate
Crystal dimensions (mm)	0.76 × 0.35 × 0.08
Crystal system	Monoclinic
Space group	$P2_1/c$
Z	4
a (Å), b (Å), c (Å)	13.5324(11), 9.8982(8), 9.7080(8)
β (°)	95.425(6)
Collection ranges	$-16 \leq h \leq 16$; $-12 \leq k \leq 12$; $-12 \leq l \leq 12$
Temperature (K)	293
Volume (Å ³)	1294.53(18)
D_x (Mg m ^{−3})	1.366
Radiation type	Mo K α ($\lambda = 0.71073$ Å)
Absorption coefficient μ (mm ^{−1})	0.10
Absorption correction	Integration
T_{max}, T_{min}	0.9909–0.9525
$F(000)$	552
θ range for data collection (°)	2.55–27.66
Independent reflections	1822 ($R_{int} = 0.113$)
Data/restraints/parameters	2682/0/185
Goodness-on-fit on F^2	1.105
Number of measured, independent, and observed [$I > 2\sigma(I)$] reflections	12087, 2682, 1822
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.116, 1.11
Largest diff. peak and hole (e Å ^{−3})	0.23 and −0.21
CCDC	1056467

chain along the c axis (Figure 2). The detail of the hydrogen bond is shown in Table 2.

3.2. Computational Methods. In order to obtain the most optimized geometry, theoretical calculations were performed

FIGURE 2: The crystal packing of the compound viewed down the c -axis.TABLE 2: Hydrogen-bond geometry of $C_{15}H_{10}N_2O_3$ ($\text{\AA}$, $^\circ$).

D-H...A	D-H	H...A	D...A	D-H...A
N2-H2A...O3 ⁱ	0.89(2)	1.99(2)	2.802(2)	151.3(19)

with ab initio HF and DFT(B3LYP) method by using the standard basis set of 6-31+G(d) [16–19] in the Gaussian03 software package [20] and Gaussview4.1 visualization program [21].

3.3. Optimized Geometry. The total energy of the title compound was calculated using the B3LYP/6-31+G(d) which is ($-912,84239530$ a.u.) lower than that calculated by the HF/6-31+G(d) method (-907.39330891 a.u.). Selected optimized parameters (bond lengths, bond angles, and torsion angles) are listed in Table 3 with related experimental and theoretical values. All of these optimized parameters are obtained from experimental X-ray analysis and theoretically calculated by HF/6-31+G (d) and B3LYP/6-31+G (d) methods. It is seen that obtained optimized parameters show a good approximation with X-ray results. But some of these optimized parameters are somewhat different from experimental values. It is because the theoretical calculations are made for isolated molecules in gaseous phase while experimental results are based on solid phase of the molecule [22, 23]. The most notable discrepancy occurs at C8-N1-N2-C9 torsion angle ($-91.2(3)^\circ$ for X-ray, -74.3417° for DFT, and -72.6382° for HF) which is partially involved in the hydrogen bond. It can be considered that intermolecular interaction affects the crystal system. The bridged C10-C9-N2-N1 torsion angle was obtained as $179.68(18)^\circ$ for X-ray results. This torsion angle has been calculated as 174.620° and 174.582° for DFT and HF levels, respectively. Root-mean-square-error (RMSE) was

obtained with selected theoretical values. Calculated RMSE for selected bond lengths and bond angles are $0.0198 \text{ \AA}$, 0.606° for B3LYP/6-31+G(d) level, and $0.0145 \text{ \AA}$, 0.753° for HF/6-31+G(d) level, respectively. As a result of these calculations, it can be interpreted that B3LYP/6-31+G(d) level is giving more consistent results with X-ray experimental values.

3.4. Molecular Electrostatic Potential (MEP). To illustrate the charge distribution of the title compound, the molecular electrostatic potential (MEP) was investigated by B3LYP function theory with the standard basis set of 6-31+G(d). Electrostatic potential, $V(r)$, that is formed by nuclei and electrons of the system at given point (r) is defined as [24]

$$V(r) = \sum_A \frac{Z_A}{|\mathbf{R}_A - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}') d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|}, \quad (1)$$

where Z_A is the charge of nucleus A that is located at $\mathbf{R}_A$, $\rho(r')$ is electron density function of molecule, and r' is the dummy integration variable. Molecular electrostatic potential (MEP) gives information of electrophilic attack and nucleophilic reactions besides hydrogen bonding interactions [25–28]. To interpret the molecular electrostatic potential (MEP) easily, a colored spectrum was used. From this spectrum the blue regions indicate positive molecular electrostatic potentials which are the preferred sites for nucleophilic attack while the red regions indicate negative molecular electrostatic potentials which are the preferred sites for electrophilic attack. As seen from Figure 3, the negative regions were mainly condensed on O atoms of the molecule with the maximum value of -0.053 a.u. for atom O3 whereas positive regions were localized on N2-H2A bond of the amide group in the studied molecule with maximum value of 0.0548 a.u. These

TABLE 3: Selected molecular parameters of $C_{15}H_{10}N_2O_3$.

	XRD	DFT	HF
Bond lengths (Å)			
N1-N2	1.381(2)	1.3716	1.359
C8-N1	1.397(3)	1.4184	1.3968
C7-N1	1.402(3)	1.4184	1.3973
C9-O3	1.225(2)	1.2201	1.194
C9-N2	1.354(3)	1.3971	1.3799
C7-O1	1.195(2)	1.2101	1.1838
C5-C6	1.371(3)	1.3888	1.3785
C1-C6	1.379(3)	1.3995	1.383
C6-C7	1.486(3)	1.4913	1.4912
C10-C11	1.374(3)	1.4038	1.3912
C10-C15	1.389(3)	1.4028	1.3912
C9-C10	1.486(3)	1.4955	1.4949
C1-C2	1.382(3)	1.389	1.3787
C1-C8	1.480(3)	1.4889	1.4889
C8-O2	1.202(3)	1.2117	1.1854
C4-C5	1.385(3)	1.4019	1.3913
C2-C3	1.388(4)	1.4019	1.3912
C3-C4	1.367(4)	1.4024	1.3923
C12-C13	1.373(4)	1.3976	1.3866
Bond angle (°)			
N2-N1-C8	123.27(18)	122.915	122.7014
N2-N1-C7	123.00(17)	122.5233	122.2112
C8-N1-C7	113.62(17)	112.7771	113.1504
C9-N2-N1	119.45(18)	118.2369	117.9273
C5-C6-C1	121.4(2)	121.4357	121.6391
O1-C7-N1	125.0(2)	125.6323	125.962
O1-C7-C6	131.0(2)	129.8207	129.4085
N1-C7-C6	104.01(17)	104.542	104.6243
O3-C9-N2	121.3(2)	121.3245	121.529
O3-C9-C10	123.18(19)	123.7278	123.3337
N2-C9-C10	115.51(19)	114.9366	115.1286
C6-C1-C8	108.91(18)	108.7184	108.4288
O2-C8-N1	125.0(2)	124.8665	125.1344
O2-C8-C1	130.6(2)	130.2991	129.9333
N1-C8-C1	104.45(18)	104.8099	104.9055
Torsion angle (°)			
C8-N1-N2-C9	-91.2(3)	-74.3417	-72.6382
C7-N1-N2-C9	84.7(3)	89.3365	90.4325
O1-C7-N1-N2	3.4(3)	11.5618	11.8452
O1-C7-N1-C8	179.7(2)	176.7365	176.3893
C6-C7-N1-N2	-176.97(18)	-169.1879	-168.9236
O3-C9-N2-N1	0.5(3)	-6.5549	-6.4589
C10-C9-N2-N1	179.68(18)	174.6203	174.5823
O2-C8-N1-N2	-1.6(3)	-12.4385	-12.8859
O2-C8-N1-C7	-177.9(2)	-177.5464	-177.3435
C1-C8-N1-N2	177.86(18)	169.2046	168.8411

values give information where the molecule tends to have hydrogen bond interactions. The obtained MEP results would help in understanding intermolecular hydrogen bond $N2-H2A \cdots O3$ which is obtained from X-ray analysis.

TABLE 4: Comparison of the experimental and calculated vibrational frequencies (cm^{-1}).

Assignments	Experiment	DFT	HF
ν (N-H)	3350	3460	3462
ν (C-H) of R_3	3100	3098	3038
ν_{as} (C-H) of R_1	3010	3061	3011
ν_s (C=O) of R_2	1790	1778	1843
ν_{as} (C=O) of R_2	1749	1734	1788
ν (C=O)	1716	1698	1750
ν_{as} (C=C) of R_3	1640	1593	1600
ν_{as} (C=C) of R_1	1601	1568	1583
γ (N-H)	1488–1530	1480	1509
ν (N-N)	1384	1373	1433
ν (C-C) + (N-H)	1284	1225	1244
ν (C-N) of R_2	1121	1083	1127
ω (N-H)	879	872	880
ω (C-H) of R_3	703	689	720
ω (C-H) of R_1	691	697	717

Note: ν , stretching; γ , rocking; ω , wagging; s, symmetric; as, asymmetric; R, ring.

FIGURE 3: Molecular electrostatic map for molecular compound, $C_{15}H_{10}N_2O_3$, calculated at B3LYP/6-31G+(d) level.

3.5. Scanning Electron Micrography (SEM). Surface morphology of the grown crystal, *N*-(1,3-dioxoisindolin-2yl)benzamide, was investigated by scanning electron microscope. SEM measurements were performed at FEI-Quanta FEG 250. The surface morphology and particle size of the title compound, $C_{15}H_{10}N_2O_3$, have been shown in Figure 4. From the SEM micrographs, it can be seen that particles have nonuniform distribution. The structural morphology consists of foam-like shape. SEM images were taken 20000x and 5000x magnifications with acceleration voltage of 3–4 kV.

3.6. IR Spectra. The experimental FTIR spectra were collected by using KBr Pellets on Schmadzu 8900 FT-IR spectrophotometer and shown in Figure 5. Obtained frequencies were recorded in wave number cm^{-1} . In this section of the study, vibrational frequencies calculated at B3LYP/6-31+G(d) and HF/6-31+G(d) levels and scaled by 0.9613 and 0.8929, respectively [29, 30]. As seen from Table 4, calculated and experimental values are in good agreement to each other. The broadest absorption was observed at 3350 cm^{-1} due to

FIGURE 4: SEM images of $C_{15}H_{10}N_2O_3$. FIGURE 5: IR spectra of $C_{15}H_{10}N_2O_3$.

the N-H stretching of bridged moiety. Theoretically this band calculated at 3460 cm^{-1} and 3462 cm^{-1} for B3YLP and HF methods, respectively. N-H stretching vibration was observed at $2500\text{--}3500\text{ cm}^{-1}$ band range with related structure [31]. Aromatic rings have the C-H stretching vibrations assigned to $3100\text{--}3000\text{ cm}^{-1}$ [32]. For the title molecule, C-H stretching vibration was observed at 3100 cm^{-1} while theoretical values have been calculated at 3098 cm^{-1} for B3YLP/6-31+G(d) and 3038 cm^{-1} for HF/6-31+G(d) methods. For the title compound, C=O symmetric stretching mode and asymmetric stretching mode were observed at 1790 cm^{-1} and 1749 cm^{-1} for dioxoisindolin group, respectively. All these experimental vibrational assignments are in agreement with related compound [33]. Calculated values of the C=O symmetric stretching mode were 1778 cm^{-1} and 1843 cm^{-1} for B3YLP and HF, respectively. These asymmetric stretching frequencies were computed at 1734 cm^{-1} and 1788 cm^{-1} for B3YLP and HF, respectively. C=O vibration of the amide group was observed at 1716 cm^{-1} experimentally. Presence of these spectroscopic values (N-H and C=O vibrations) shows that the title molecule has ketoamine tautomeric form [34, 35]. The details of the spectral values are shown in Table 4.

4. Conclusions

In this paper we have investigated the molecular structure of *N*-(1,3-dioxoisindolin-2-yl)benzamide, using single crystal X-ray diffraction, IR spectroscopy, and computational

methods. The results obtained show that the X-ray crystal structure and computational methods are consistent with each other. There was particularly good agreement using the DFT (B3LYP) with the 6-31+G(d) basis set. The structural X-ray analysis has indicated that the crystal structure is stabilized by N-H $\cdots$ O hydrogen bonding. These results were consistent with those obtained by a MEP analysis. The calculated and observed N-H and C=O vibrations in the IR spectrum confirm the ketoamine tautomeric form of the structure. The surface morphology was also studied by SEM analysis and the results indicate a nonuniform distribution for the sample.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

References

- [1] B. K. Revathi, D. Reuben Jonathan, S. Sathya, K. Prathebha, and G. Usha, "Crystal structure of 4-methyl-*N*-[2-(piperidin-1-yl)ethyl]benzamide monohydrate," *Acta Crystallographica Section E Crystallographic Communications*, vol. 71, no. 5, pp. o359–o360, 2015.
- [2] S. A. Prabhu, M. Suresh, A. A. Jameel, M. S. A. Padusha, and B. Gunasekaran, "Crystal structure of *N*-[(morpholin-4-yl)(thiophen-2-yl)methyl]benzamide," *Acta Crystallographica E*, vol. 71, pp. o498–o499, 2015.
- [3] J. J. Novina, G. Vasuki, A. Baheti, and K. R. J. Thomas, "*N*-(4,4'-Dibromo-[1,1'-biphenyl]-2-yl)benzamide," *Acta Crystallographica Section E: Structure Reports Online*, vol. 69, no. 2, article o222, 2013.
- [4] K. Chowdhury, R. Mukhopadhyay, M. Mukherjee, C. K. Broder, and G. Kundu, "(*Z*)-3-Acetonilidene-2,3-dihydro-1*H*-isindolin-1-one," *Acta Crystallographica Section E*, vol. 57, pp. o421–o423, 2001.
- [5] I. Pendrak, S. Barney, R. Wittrock, D. M. Lambert, and W. D. Kingsbury, "Synthesis and anti-HSV activity of a ring-deleted mappicine ketone analog," *Journal of Organic Chemistry*, vol. 59, no. 9, pp. 2623–2625, 1994.
- [6] E. C. Taylor, P. Zhou, L. D. Jennings, Z. Mao, B. Hu, and J.-G. Jun, "Novel synthesis of a conformationally-constrained analog of DDATHF," *Tetrahedron Letters*, vol. 38, no. 4, pp. 521–524, 1997.
- [7] G. Pandey, R. Varkhedkar, and D. Tiwari, "Efficient access to enantiopure 1,3-disubstituted isindolines from selective catalytic fragmentation of an original desymmetrized rigid

- overbred template," *Organic & Biomolecular Chemistry*, vol. 13, no. 15, pp. 4438–4448, 2015.
- [8] STOE & Cie, *X-AREA (Version 1.18) and X-RED32 (Version 1.04)*, STOE & Cie, Darmstadt, Germany, 2002.
 - [9] G. M. Sheldrick, "A short history of SHELX," *Acta Crystallographica Section A*, vol. 64, no. 1, pp. 112–122, 2008.
 - [10] L. J. Farrugia, "ORTEP-3 for windows—a version of ORTEP-III with a Graphical User Interface (GUI)," *Journal of Applied Crystallography*, vol. 30, no. 1, p. 565, 1997.
 - [11] L. J. Farrugia, "WinGX suite for small-molecule single-crystal crystallography," *Journal of Applied Crystallography*, vol. 32, no. 4, pp. 837–838, 1999.
 - [12] S. K. Mohamed, M. A. Farrukh, M. Akkurt, M. R. Albayati, and A. A. Abdelhamid, "2-(1,3-Dioxoisindolin-2-yl)acetic acid-*N'*-[(*E*)-2-methoxybenzylidene]pyridine-4-carbohydrazide (1/1)," *Acta Crystallographica E*, vol. 68, p. o2442, 2012.
 - [13] M. H. Bhatti, U. Yunus, S. Saeed, S. R. Shah, and W.-T. Wong, "The 1:1 adduct of caffeine and 2-(1,3-dioxoisindolin-2-yl)acetic acid," *Acta Crystallographica Section E*, vol. 67, no. 9, Article ID o2240, 2011.
 - [14] W. Sripet, S. Chantrapromma, P. Ruanwas, and H.-K. Fun, "4-Bromo-*N*-(4-methoxy-2-nitrophenyl)benzamide," *Acta Crystallographica Section E: Structure Reports Online*, vol. 68, no. 4, Article ID o1234, 2012.
 - [15] J. Bernstein, R. E. Davies, L. Shimoni, and N.-L. Chang, "Patterns in hydrogen bonding: functionality and graph set analysis in crystals," *Angewandte Chemie*, vol. 34, no. 15, pp. 1555–1573, 1995.
 - [16] A. D. Becke, "Density-functional thermochemistry. III. The role of exact exchange," *The Journal of Chemical Physics*, vol. 98, no. 7, pp. 5648–5652, 1993.
 - [17] C. Lee, W. Yang, and R. G. Parr, "Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density," *Physical Review B*, vol. 37, no. 2, pp. 785–789, 1998.
 - [18] H. B. Schlegel, "Optimization of equilibrium geometries and transition structures," *Journal of Computational Chemistry*, vol. 3, no. 2, pp. 214–218, 1982.
 - [19] C. Peng, P. Y. Ayala, H. B. Schlegel, and M. J. Frisch, "Using redundant internal coordinates to optimize equilibrium geometries and transition states," *Journal of Computational Chemistry*, vol. 17, no. 1, pp. 49–56, 1996.
 - [20] M. J. Frisch, G. W. Trucks, H. B. Schlegel et al., *Gaussian 03, Revision E.01*, Gaussian, Wallingford, Conn, USA, 2004.
 - [21] R. Dennington, T. Keith, and J. Millam, *GaussView, Version 4.1*, Semichem, Shawnee Mission, Kan, USA, 2007.
 - [22] B. Gonzales, P. Lorenzo-Luis, A. Romerosa, M. Serrano-Ruiz, and P. Gili, "Theoretical aspects on water soluble $[\text{RuClCp}(\text{PPh}_3)_2]$, $[\text{RuClCp}(\text{PTA})(\text{PPh}_3)]$, $[\text{RuClCp}(\text{PTA})_2]$, $[\text{RuClCp}(\text{mPTA})(\text{PPh}_3)]^+$ and $[\text{RuClCp}(\text{mPTA})_2]^{2+}$ (PTA = 1,3,5-triaza-7-phosphaadamantane; mPTA = *N*-methyl-1,3,5-triaza-7-phosphaadamantane)," *Journal of Molecular Structure: THEOCHEM*, vol. 894, pp. 59–63, 2009.
 - [23] P. D. S. Babu, S. Perianthy, S. Mohan, S. Ramalingam, and B. G. Jayaprakash, "Molecular structure and vibrational investigation of benzenesulfonic acid methyl ester using DFT (LSDA, B3LYP, B3PW91 and MPW1PW91) theory calculations," *Spectrochimica Acta—Part A: Molecular and Biomolecular Spectroscopy*, vol. 78, no. 1, pp. 168–178, 2011.
 - [24] P. Politzer and J. S. Murray, "The fundamental nature and role of the electrostatic potential in atoms and molecules," *Theoretical Chemistry Accounts*, vol. 108, no. 3, pp. 134–142, 2002.
 - [25] E. Scrocco and J. Tomasi, "Electronic molecular structure, reactivity and intermolecular forces: an heuristic interpretation by means of electrostatic molecular potentials," in *Advances in Quantum Chemistry*, vol. 11, pp. 115–121, Elsevier, 1978.
 - [26] F. J. Luque, J. M. Lopez, and M. Orozco, "Perspective on 'Electrostatic interactions of a solute with a continuum. A direct utilization of ab initio molecular potentials for the prevision of solvent effects,'" *Theoretical Chemistry Accounts*, vol. 103, pp. 343–345, 2000.
 - [27] H. Tanak, F. Erşahin, Y. Köysal, E. Ağar, Ş. Işık, and M. Yavuz, "Theoretical modeling and experimental studies on *N*-*n*-Decyl-2-oxo-5-nitro-1-benzylidene-methylamine," *Journal of Molecular Modeling*, vol. 15, no. 10, pp. 1281–1290, 2009.
 - [28] H. Saraçoğlu, Ö. Sariöz, and S. Öznergiz, "Quantum chemical, spectroscopic, and X-ray diffraction studies of *N*-diphenylphosphino-4-methylpiperidine selenide (1)," *Molecular Crystals and Liquid Crystals*, vol. 591, no. 1, pp. 47–63, 2014.
 - [29] J. B. Foresman and A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc, Pittsburgh, Pa, USA, 2nd edition, 1996.
 - [30] J. P. Merrick, D. Moran, and L. Radom, "An evaluation of harmonic vibrational frequency scale factors," *Journal of Physical Chemistry A*, vol. 111, no. 45, pp. 11683–11700, 2007.
 - [31] Ç. Yüksektepe, N. Çalışkan, M. Genç, and S. Servi, "Synthesis, crystal structure, HF and DFT calculations of 1-(2-chlorobenzyl)-*N*-(1-(2-chlorobenzyl)-4,5-dihydro-1*H*-imidazol-2-yl)-1*H*-benzimidazol-2-amine," *Crystallography Reports*, vol. 55, no. 7, pp. 1188–1193, 2010.
 - [32] K. Sarojini, H. Krishnan, C. C. Kanakam, and S. Muthu, "Synthesis, structural, spectroscopic studies, NBO analysis, NLO and HOMO–LUMO of 4-methyl-*N*-(3-nitrophenyl)benzene sulfonamide with experimental and theoretical approaches," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 108, pp. 159–170, 2013.
 - [33] K. Faghihi, M. Absalar, and M. Hajibeygi, "Synthesis and characterization of new optically active polyamides containing 2-(4-nitro-1,3-dioxoisindolin-2-yl)succinic acid and aromatic diamines via direct polycondensation," *Turkish Journal of Chemistry*, vol. 34, pp. 81–90, 2010.
 - [34] A. Elmalı, M. Kabak, E. Kavlakoglu, Y. Elerman, and T. N. Durlu, "Tautomeric properties, conformations and structure of *N*-(2-hydroxy-5-chlorophenyl) salicylaldehyde," *Journal of Molecular Structure*, vol. 510, no. 1–3, pp. 207–214, 2000.
 - [35] S. R. Salman and N. A. I. Saleh, "Infra-red study of tautomerism in some schiff bases," *Spectroscopy Letters*, vol. 30, no. 7, pp. 1289–1300, 1997.