Contents lists available at SciVerse ScienceDirect



Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy



journal homepage: www.elsevier.com/locate/saa

Experimental and quantum chemical computational study of (*E*)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone

Serap Yazıcı^{a,*}, Çiğdem Albayrak^b, İsmail Erdem Gümrükçüoğlu^c, İsmet Şenel^a, Orhan Büyükgüngör^a

^a Department of Physics, Ondokuz Mayıs University, Samsun 55139, Turkey

^b Department of Science Education, Sinop University, Sinop, Turkey

^c Department of Chemistry, Ondokuz Mayıs University, Samsun, Turkey

ARTICLE INFO

Article history: Received 14 October 2011 Received in revised form 18 February 2012 Accepted 23 February 2012

Keywords: Crystal structure Diazenyl Density functional theory (DFT) Conformational analysis Non-linear optical properties (NLO) Solvent media

ABSTRACT

In this work, the azo dye, (*E*)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone, has been synthesized and characterized by IR, and X-ray single-crystal determination. In the theoretical calculations, the stable structure geometry of the isolated molecule in gas phase was investigated under the framework of the density functional theory (B3LYP) with 6-31G (d, p). To designate lowest energy molecular conformation of the title molecule, the selected torsion angle was varied every 10° and the molecular energy profile was calculated from -180° to $+180^{\circ}$. Besides, molecular electrostatic potential (MEP), frontier molecular orbitals (FMO) analysis, and thermodynamic properties were described from the computational process. In addition to these calculations, we were investigated solvent effects on the nonlinear optical properties (NLO) of the title compound.

© 2012 Elsevier B.V. All rights reserved.

1. Introduction

It is well known that azo dyes play an important role in dyes and pigments industry. They have been most widely used in fields such as dyeing textile fiber, biomedical studies, advanced applications in organic synthesis and high technology areas like lasers, electro-optical devices, and ink-jet printers [1–3]. In addition, azobenzene and its derivatives have attracted much attention for their nonlinear optical properties [4–6]. Azo dyes contain at least one chromophoric azo group (-N=N-), links two sp² hybridized C atoms, attached to the substituents. The low-lying azo centered π^* molecular orbital is responsible for the intense long-wavelength absorption (dye function) and the nonlinear optical properties (information storage function) [7].

Here, we wish to report the synthesis crystal and molecular structure of the dye derived from 2-hydroxyacetophenone: (E)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone by IR and X-ray determination. The conformational analysis of the title molecule with respect to the selected torsion angle is achieved by DFT. Besides these, the molecular structure and geometry, FMOs, MEP, thermodynamic properties have also been studied and investigated that the optical response of the title molecule in the solvent media with the computational studies.

2. Experimental and computational methods

2.1. Instrumentation

The FT-IR spectrum of the title compound was recorded in the 4000–400 $\rm cm^{-1}$ region with a Bruker Vertex 80 V FT-IR spectrometer using KBr pellets.

2.2. Synthesis

The compound was prepared by reflux a mixture of 3,4-dimethylaniline (0.944 g, 7.8 mmol), water (20 ml) and concentrated hydrochloric acid (1.97 ml, 23.4 mmol) was stirred until a clear solution was obtained. This solution was cooled down to $0-5 \,^{\circ}$ C and a solution of sodium nitrite (0.75 g, 7.8 mmol) in water was added dropwise while the temperature was maintained below $5 \,^{\circ}$ C. The resulting mixture was stirred for 30 min in an ice bath. 2-Hydroxyacetophenone (1.067 g, 7.8 mmol solution (pH 9) was gradually added to a cooled solution of 3,4-dimethylbenzenediazonium chloride, prepared as described above, and the resulting mixture was stirred at $0-5 \,^{\circ}$ C for 2 h in ice bath. The product was recrystallized from ethyl alcohol to obtain solid (*E*)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone.

Crystals of (*E*)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone were obtained after one day by slow evaporation from acetic acid (yield 78%, m.p. = 405-407 K).

^{*} Corresponding author. Tel.: +90 362 3121919x5285; fax: +90 362 4576092. *E-mail address*: yserap@omu.edu.tr (S. Yazıcı).

^{1386-1425/\$ –} see front matter 0 2012 Elsevier B.V. All rights reserved. doi:10.1016/j.saa.2012.02.092

Table 1

Crystal data and structure refinement parameters for the title compound.

Chemical formula	$C_{16}H_{16}N_2O_2$
Color/shape	Brown/prism
Formula weight	268.31
Temperature	150 K
Crystal system	Triclinic
Space group	P-1
Unit cell parameters	a = 7.1429(4)Å
	b=9.9121(7)Å
	c=10.0125(6)Å
	$\alpha = 93.345(5)^{\circ}$
	$\beta = 102.297(5)^{\circ}$
	$\gamma = 91.957(5)^{\circ}$
Volume	690.67(8)Å ³
Ζ	2
Density	1.291 g/cm ³
Absorption coefficient	$0.086 \mathrm{mm^{-1}}$
T _{min} , T _{max}	0.9698, 0.9893
Diffractometer/meas. meth.	STOE IPDS $2/\varpi$ -scan
heta range for data collection	2.83° to 26.50°
Unique reflections measured	11,629
Independent/observed reflections	2857/1924
Data/restraints/parameters	1924/0/209
Goodness of fit on F ²	1.090
Final <i>R</i> indices $[I > 2\sigma(I)]$	$R_1 = 0.0543, wR_1 = 0.1256$
R indices (all data)	$R_2 = 0.0857, wR_2 = 0.1400$

2.3. Crystal data for the title compound

A brown crystal of the compound with dimensions $0.53 \text{ mm} \times 0.32 \text{ mm} \times 0.14 \text{ mm}$ was mounted on goniometer and data collection was performed on a STOE IPDS II diffractometer by the ω scan technique using graphite-monochromatic Mo K_{α} radiation (λ = 0.71073 Å) at room temperature (296 K). Unit cell parameters were determined from least-squares refinement of setting angels with θ in the range 2.83 $\leq \theta \geq$ 26.50. The refinement was carried out by full-matrix least-squares method on the positional and anisotropic temperature parameters of the non-hydrogen atoms, or equivalently corresponding to 209 crystallographic parameters. Atom H1 was located in a difference Fourier map and refined isotropically, and the other H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.93 Å and 0.96 Å for aromatic CH and CH₃ atoms, respectively. The displacement parameters of the H atoms were fixed at $U_{iso}(H) = 1.2U_{eq}(C)$ (1.5U_{eq} for methyl) of their parent atoms. For the title compound data collection and cell refinement: X-AREA [8]; data reduction: X-RED32 [8]; program used to solve structure: SHELXS 97 [9]; program used to refine structure: SHELXL 97 [9]; molecular figure: ORTEP III [10] publication software: WinGX [11]. Details of the data collection conditions and the parameters of the refinement process are given in Table 1.

2.4. Computational procedure

The molecular structure of the title molecule is optimized by the DFT calculations with a hybrid functional B3LYP (Becke's Three parameter Hybrid Functional using the LYP Correlation Functional) at 6-31G (d, p) basis set [12,13] and all of the calculations were carried out using Gaussian 03 program package [14]. The vibrational frequencies of the optimized molecule have also been calculated at the same level of the theory and achieved frequencies were scaled by 0.9627 [15]. To elucidate conformational features of the molecule, the selected degree of torsional freedom, T (C6–C1–N1–N2), was varied from -180° to $+180^{\circ}$ in every 10° and the molecular energy profile was obtained with the B3LYP/6-31G (d, p) method. In addition, FMO's, MEP and thermodynamic properties were performed with the same level of theory. To investigate



Fig. 1. ORTEP III diagram of the title compound.

the effect of solvent on the energetic behavior and NLO properties of the title molecule, the PCM (polarizable continuum model) [16] was employed by B3LYP/6-31G (d, p).

3. Results and discussion

3.1. Description of the crystal structure

The molecular structure of (E)-1-[5-(3,4dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone with the atom numbering scheme is shown in Fig. 1 and selected geometric parameters are given in Table 2. The title compound crystallizes in the triclinic space group P-1 with two molecules (Z=2) in the unit cell. The compound has two aromatic rings and an azo moiety. In the molecule, the benzene rings which linked to azo bridge adopt trans configuration with respect to the N=N double bond. The title molecule is almost coplanar, making a dihedral angle between the aromatic rings of $1.83(1)^{\circ}$. In the title compound, the C1-N1-N2-C9 torsion angle is 180(2)° as a result of the partial electron delocalization on the azo bridge. It is expected that C6-C1-N1 and C14-C9-N2 angles are 120° since C1 and C2 atoms have sp^2 hybridization. Due to the steric effect between the azo moiety and substitute groups, these angles have been deviated from 120° with dihedral angle of $116.7(2)^{\circ}$, $115.7(2)^{\circ}$, respectively. The most important bonds of the azo compounds are N1=N2, C1-N1 and N2-C9 and values of them are 1.254(3)Å, 1.428(3)Å and 1.424(3)Å, respectively and these bond lengths are in a good agreement with found of those in the literature [17,18]. Furthermore, C7-O2 and C4-O1 bonds which have distance of 1.233(3)Å, 1.349(3)Å, respectively, are also compared well with the values reported previously [19].

In the title azo dye, there is a strong intramolecular O–H··O hydrogen bond which generates S(6) ring motif [20]. The sum of the van der Waals radii of the two O atoms (3.04 Å) is significantly longer than the intramolecular O···O hydrogen bond length [21]. The crystal packing is stabilized by van der Waals interactions and the details of the intramolecular hydrogen bond are summarized in Table 2.

3.2. Optimized geometry and conformational analysis

Selected structural parameters obtained experimentally and calculated theoretically using B3LYP with the 6-31G (d, p) basis set are tabulated in Table 3 as comparative. The optimized parameters by DFT show a small difference from those obtained by

Table 2 Hydrogen-bond geometry (Å,°).

D—H···A	D—H	H···A	$D{\cdot}{\cdot}{\cdot}A$	D—H…A
01-H1···02	0.91(3)	1.70(3)	2.544(2)	152(3)

Table 3

Selected molecular structure parameters for the title compound.

	X-ray	DFT
C7-02	1.233(3)	1.24196
C4-01	1.349(3)	1.33313
N1-C1	1.428(3)	1.41173
N1-N2	1.254(3)	1.26311
N2-C9	1.424(3)	1.41539
C7–C8	1.488(4)	1.51346
C12-C15	1.508(3)	1.50852
C13-C16	1.515(3)	1.50992
01-C4-C3	117.9(2)	118.11439
01-C4-C5	121.7(2)	122.21741
C5-C7-C8	120.6(2)	120.26315
C6-C1-N1	116.7(2)	115.98414
C14-C9-N2	115.7(2)	115.43609
01-C4-C5-C7	-0.2(4)	0.00224
C4-C5-C7-C8	178.0(2)	-180.00000
C15-C12-C13-C16	0.8(4)	-0.00255
C2-C1-N1-N2	1.1(3)	-0.01630
N1-N2-C9-C10	0.0(4)	-0.00526
C6-C1-N1-N2	-178.45(1)	179.98452

X-ray diffraction. It is not suprising, because the DFT calculations ignore molecular interactions. The largest difference between the experimental observations and those obtained from the theoretical calculations is 0.02546 Å for bond lengths and 0.71586° for bond angles. On the other hand, the root mean square error (RMSE) is detected about 1.3×10^{-2} Å for bond lengths. When the experimentally observed and theoretically calculated geometries are superimposed (Fig. 2), RMSE is found to be about 4.7×10^{-2} Å. This RMSE value support that there is the conformational harmony between the observed and calculated geometries. In addition to these, in the optimized molecule, the dihedral angle between the aromatic rings found to be 0° .

In order to determine the most favourable conformation as theoretically, the energy profile of the title compound as a function of C6–C1–N1–N2 torsion angle was obtained from B3LYP/6-31G (d, p) method (Fig. 3). Selected torsion angle, *T* (C6–C1–N1–N2), is $-178.45(1)^{\circ}$ for X-ray and 179.98452° for DFT-optimized geometry. The energy profile shows two maxima at $\pm 90^{\circ}$ and three minima at 0° and $\pm 180^{\circ}$. The hydroxyl attached ring perpendicular to the plane of the other aromatic ring at two maxima values of selected torsion angle. The two energy barriers arise from the steric interactions between the two aromatic rings. In the gas phase, it is clear that the most stable conformers must have a minima value of selected torsion angle and these minima are 0° and $\pm 180^{\circ}$. The optimized crystal structure has a planar conformation at these values of the torsion angle.







Fig. 3. Molecular energy profile using DFT against the selected torsional degree of freedom.

3.3. Vibrational spectra

The harmonic vibrational frequencies for the title azo dye have been calculated by using DFT method at 6-31G (d, p) level. It is known that there is a systematic error in the calculated harmonic vibrational frequency when it is compared to the experimental fundamental vibrational frequency [22]. The reason for this is the incorrect description of the electron–electron interaction and the neglect of anharmonicity in the theoretical calculations. In order to compare the theoretical results with experimental values of those, scaling factor which is 0.9627 for B3LYP/6-31G (d, p) is applied to all of the calculated frequencies. In Fig. 4, the theoretical spectrum is not scaled for the qualitative comparison.

Some of the characteristic frequencies for the title compound have given in Table 4 and the correlation graphic which described harmony between the calculated and experimental frequencies are plotted (Fig. 5). As can be seen from Fig. 5, experimental fundamentals have a better correlation with B3LYP. The experimental frequencies are slightly lower than the calculated values for the title molecule. Two factors may be responsible for the discrepancies between the experimental and theoretical spectra. The first is caused by the environment and the second reason for these discrepancies is the fact that the theoretical calculations neglect the anharmonicity effects [23]. In the experimental IR results, O–H stretching band was observed at 2000–3000 cm⁻¹ as a broad peak due to the strong intramolecular O–H···O hydrogen bond. Its value obtained by DFT calculations is 3101 cm⁻¹. While the N=N and C=O stretching vibrations were seen at 1420 cm⁻¹ and 1643 cm⁻¹, respectively, the same bands were calculated as 1495 cm⁻¹ and 1648 cm⁻¹, respectively. These stretching modes are consistent with those reported in the literature [24–26].

Table 4

Characteristic IR absorption bands of the title molecule.

Assignments	Experimental (cm ⁻¹)	Calculated (cm ⁻¹)
νΟ-Η	2000-3000	3101
ν C= 0	1643	1648
νN=N	1420	1495
νC-0	1242	1293
δ0-Н	1327	1391
vC-C	1606-1574	1605-1558
γ0-Н	626-780	862
γ C–H(ring)	829	831

 ν ; stretching, δ ; in-plane bending, γ ; out-of-plane bending



Fig. 4. Experimental (red) and calculated (black) IR spectra of the title molecule. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

3.4. Molecular electrostatic potential

The electrostatic potential at any point, $V(\mathbf{r})$, is the energy required to bring a single positive charge from infinity to that point. As each pseudo atom in the refined model consists of the nucleus and the electron density distribution described by the multipole expansion parameters, the electrostatic potential may be calculated by the evaluation of

$$V(r) = \sum_{A} \frac{Z_{A}}{|R_{A} - r|} - \int \frac{\rho(r')dr'}{|r' - r|}$$
(1)

where Z_A is the charge on nucleus A located at R_A . V(r) is a physical observable, which can be determined experimentally, by

diffraction methods, as well as computationally [27,28]. Its sign in a given region depends upon whether the positive contribution of the nuclei or the negative one of the electrons is dominant there [29]. Thus possible sites for electrophilic or nucleophilic attack may easily be identified, and a measure of the interaction of the molecule with its environment obtained.

To predict reactive sites for electrophilic attack, molecular electrostatic potential (MEP) was calculated at the B3LYP/6-31G (d, p) optimized geometry and demonstrated in Fig. 6. It is known that the negative (red) and the positive (blue) regions of the MEP represent to regions which prone to electrophilic and nucleophilic attack, respectively. As can be seen from Fig. 6, there are two negative regions localized on the O1 and O2



Fig. 5. Correlation graphic of calculated and experimental frequencies of the title compound.



Fig. 6. Molecular electrostatic potential map calculated at B3LYP/6-31G (d, p) level.



Fig. 7. Molecular orbital surfaces and energies for the HOMO and LUMO of the title compound.

Table 5

Theoretical energies (eV), dipole moments (Debye), molecular polarizabilities ($Å^3$) and hyperpolarizabilities ($\times 10^{-30}$ esu) in different media of the title compound.

Media	$Gas(\varepsilon = 1)$	Chloroform (ε = 4.711)	Ethanol (ε = 24.852)	Water (<i>ε</i> = 78.355)
Е	-23,927.315	-23,927.549	-23,927.640	-23,927.674
μ	3.5913	4.6350	4.8891	4.9400
α	34.853062	43.031982	46.221860	47.043659
β	7.5389	13.4813	17.1427	18.5744
ΔE^{a}	3.6942	3.6634	3.6484	3.6408

^a $\Delta E = E_{HOMO} - E_{LUMO}$.

atoms with values around -0.0348 and -0.0374 a.u., respectively. These are the most preferred regions for any electrophilic attack on the whole molecule. So, these regions indicate that the intramolecular hydrogen bond formed between the O1 and O2 atoms.

3.5. Frontier molecular orbitals

The highest occupied molecular orbitals (HOMOs) and the lowest-lying unoccupied molecular orbitals (LUMOs) are named as frontier molecular orbitals (FMOs). The energy gap between the HOMO and LUMO is very important in determining the chemical activity of the molecule. A small HOMO-LUMO energy gap implies low kinetic stability, because it is energetically favourable to add electrons to a low-lying LUMO and to receive electrons from a high-lying HOMO [30-32]. The distributions of the HOMO and LUMO orbitals computed at the B3LYP/6-31G (d, p) level for the title molecule and illustrated in Fig. 7. As can be clearly seen from the figure, HOMO and LUMO orbitals are extended over the entire molecule. The energy difference between the HOMO and LUMO was obtained as 3.6942 eV in the gas phase calculations. With this energy gap, it can be said that the title molecule has high kinetic stability and low chemical reactivity as in our previous study [26].

3.6. The solvent effect on the nonlinear optical properties

Nonlinear optical (NLO) effects arise from the interactions of electromagnetic fields in various media to produce new fields altered in phase, frequency, amplitude or other propagation characteristics from the incident fields. The molecules, exhibiting efficient nonlinear optical properties, have been investigated intensively because of their potential applications in telecommunication, data storage and optical signal processing [33–39]. The theoretical and experimental works clearly shows that the environment plays a remarkable role in the considerations of the first- and the second-order hyperpolarizabilities of the molecules. On the other hand, the linear polarizability is less affected by the solvent than the higher order polarizabilities [40].

In order to inspect the effects of solvent on (hyper) polarizabilities, the NLO properties of the title molecule were calculated at B3LYP/6-31G (d, p) level by adding the self-consistent reaction field (SCRF) approach with polarizable continuum model (PCM) [41,42]. In different solvents (chloroform, ethanol, water) energy, dipole moment, (hyper) polarizability and the HOMO-LUMO energy gap of the title compound are tabulated in Table 5. As can be seen from the table, with increasing polarity of the solvent, a decline was observed for the HOMO-LUMO energy gap of the title azo dve. On the other hand, dipole moment, polarizability and hyperpolarizability of the title molecule were raised with polarity of the solvent. As the HOMO-LUMO energy range decreases, the electrons are more easily excited from the HOMO to the LUMO and the electronic charge asymmetry of the molecule can be easily changed when the external electric field is applied. So, with polarity of the solvent, the increment of polarizability and hyperpolarizability values of the title compound is not surprising for this study. In addition to these, together with the increasing polarity of the solvent, the stability of the title compound decreases in going to the solution phase.

3.7. Thermodynamic properties

Based on the vibrational analysis at B3LYP/6-31G (d, p) level and statistical thermodynamics, the standard thermodynamic functions: heat capacity ($C_{p,m}^{0}$), entropy (S_{m}^{0}), and enthalpy (H_{m}^{0}) were obtained at constant pressure (Table 6) and at constant temperature (Table 7).

Table 6
Thermodynamic properties at different temperatures at B3LYP/6-31G (d, p) level

T(K)	$H_m^0(ext{kcal mol}^{-1})$	$C_{p,m}^0({\rm cal}\ {\rm mol}^{-1}{\rm K}^{-1})$	$S_m^0({\rm cal}\ {\rm mol}^{-1}\ {\rm K}^{-1})$
100	1.910	28.955	88.527
200	6.049	49.733	116.395
298.15	12.133	70.293	140.870
300	12.267	70.680	141.319
400	20.551	90.688	165.013
500	30.709	107.984	187.609

Table 7 Thermodynamic properties at different pressures at B3LYP/6-31G (d, p) level.

P(atm)	$H_m^0(ext{kcal mol}^{-1})$	$C_{p,m}^{0}(\text{cal mol}^{-1} \text{ K}^{-1})$	$S_m^0({\rm cal}\ { m mol}^{-1}\ { m K}^{-1})$
1 1.5 2 2.5 3 3.5 4 4.5 5	12.133 Con- stant	70.293 Con- stant	140.870 140.065 139.493 139.050 138.687 138.381 138.116 137.882 137.672

As seen from Table 6, the standard thermodynamic functions increase with increasing temperature, due to the intensities of molecular vibration increase as temperature increase. While the pressure is increased at 298.15 K, it was observed that the entropy increases but the enthalpy and the heat capacity remain constant (Table 7). According to Boyle's Law for gases, a molecule is compressed at constant temperature its volume decreases [43]. Due to decreasing volume, the number of possible sites that occupied by particles of the molecule may be restricted. Thus, the entropy tends to decrease with increasing pressure at constant temperature. This investigation will be helpful for the further studies of the title molecule.

4. Conclusion

In this study, we investigated molecular and structural of (E)-1-[5-(3,4-dimethylphenyldiazenyl)-2properties hydroxyphenyllethanone with X-ray diffraction and FT- IR as well as DFT calculations. The comparison between the calculated results and the X-ray experimental data indicate that B3LYP/6-31G (d, p) method shows a good agreement with the experimental results. There are some differences between the theoretical and experimental frequencies. The differences related to the weakening of the OH bond due to the intra-molecular hydrogen bonding. Generally, we can say that there is a good linear correlation between them. The MEP map shows that there are two negative regions around the oxygen atoms. These sites allow researchers to predict the most probable hydrogen bonding in the molecule. In the solvent media, while the HOMO-LUMO energy gap of the molecule is decreased the (hyper) polarizability and dipole moment values are increased. So, in the present study, NLO parameters display an increment in the solvent media. The title compound is stable in the gas phase more than in polar solvents. The thermodynamic properties of the title compound were also obtained at constant temperature and at constant pressure. We hope that our paper will be helpful for new researchers are working on the organic molecules.

Acknowledgements

The authors wish to acknowledge the Faculty of Arts and Sciences, Ondokuz Mayis University, Turkey, for the use of STOE IPDS 2 diffractometer (purchased under grant F.279 of the University Research Fund).

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.saa.2012.02.092.

References

- A.T. Peters, H.S. Freeman, Colour Chemistry, the Design and Synthesis of Organic Dyes and Pigments, Elsevier Appl Sci Publ Ltd, Barking, Essex, 1991.
- [2] P. Gregory, High-technology Applications of Organic Colorants, Plenum Press, New York and London, 1991.
- [3] S.C. Catino, R.E. Farris, Azo Dyes, John Wiley & Sons, New York, 1985.
- [4] Z. Sekkat, M. Dumont, Appl. Phys. B 54 (1) (1992) 486-489.
- [5] T. Ikeda, O. Tsutsumi, Science 268 (1995) 1873-1875.
- [6] R.H. Berg, S. Hvlisted, P.S. Ramanujam, Nature 383 (1996) 505-508.
- [7] M. Snehalatha, C. Ravikumar, I. Hubert Joe, N. Sekar, V.S. Jayakumar, Spec-
- trochim. Acta A 72 (2009) 654–662. [8] Stoe & Cie, X-AREA (Version 1.18) and X-RED32 (Version 1.04), Darmstadt, Germany, 2002.
- [9] G.M. Sheldrick, Acta Crystallogr. A 64 (2008) 112-122.
- [10] L.J. Farrugia, J. Appl. Cryst. 30 (1997) 565.
- [11] L.J. Farrugia, J. Appl. Cryst. 32 (1999) 837-838.
- [12] A.D. Becke, J. Chem. Phys. 98 (1993) 5648-5652.
- [13] C. Lee, W.T. Yang, R.G. Parr, Phys. Rev. B 37 (1) (1988) 785-789.
- [14] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatjim, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian 03W, Revision E. 01, Wallingford, CT, Gaussian Inc, 2004.
- [15] J.P. Merrick, D. Moran, L. Radom, J. Phys. Chem. A 111 (1) (2007) 11683-11700.
- [16] J. Tomasi, B. Mennucci, R. Cammi, Chem. Rev. 105 (2005) 2999–3093.
- [17] T.S.B. Baul, S. Kundu, H.D. Arman, E.R.T. Tiekink, Acta Crystallogr. E 65 (2009) o3061-o3306.
- [18] M.R. Han, D. Hashizume, M. Hara, Acta Crystallogr. E 62 (2006) o3001-o3003.
- [19] H. Karabıyık, H. Petek, N.O. İskeleli, Ç. Albayrak, Struct. Chem. 20 (2009) 903-910.
- [20] J. Bernstein, R.E. Davis, L. Shimoni, N.L. Chang, Angew. Chem. Int. Ed. Engl. 34 (1995) 1555–1573.
- [21] A. Bondi, J. Phys. Chem. 68 (1964) 441-452.
- [22] A.P. Scott, L. Radom, J. Phys. Chem. 100 (1996) 16502-16513.
- [23] H.A. Dabbagh, A. Teimouri, A.N. Chermahini, M. Shahraki, Spectrochim. Acta A 69 (2008) 449–459.
- [24] C. Albayrak, I.E. Gümrükçüoğlu, M. Odabaşoğlu, N.O. İskeleli, E. Ağar, J. Mol. Struct. 932 (2009) 43–54.
- [25] R.M. Silverstein, F.X. Webster, D. Kiemle, J. Spectrometric Identification of Organic Compounds, seventh ed., John Wiley & Sons, New York, 2005.
- [26] S. Yazıcı, Ç. Albayrak, I.E. Gümrükçüoğlu, İ. Şenel, O. Büyükgüngör, J. Mol. Struct. 985 (2011) 292–298.
- [27] R.F. Stewart, Chem. Phys. Lett. 65 (1979) 335–342.
- [28] P. Politzer, D.G. Truhlar, Chemical Applications of Atomic and Molecular Electrostatic Potentials, Plenum, New York, 1981
- [29] P. Politzer, P. Lane, J.S. Murray, Cent. Eur. J. Ener. Mater. 8 (2011) 39-52.
- [30] M.D. Diener, J.M. Alford, Nature 393 (1998) 668-671.
- [31] S.H. Yang, C.L. Pettiette, J. Conceicao, O. Cheshnovsky, R.E. Smalley, Chem. Phys. Lett. 139 (1987) 233–238.
- [32] H. Handschuh, G. Ganteför, B. Kessler, P.S. Bechthold, W. Eberhardt, Phys. Rev. Lett. 74 (1995) 1095–1098.
- [33] D.S. Chemia, J. Zyss, Nonlinear Optical Properties of Organic Molecules and Crystals, Academic, New York, 1987.
- [34] M.D. Aggarwal, J. Stephens, A.K. Batra, R.B. Lal, J. Optoelectron. Adv. Mater. 5 (2003) 555–562.
- [35] R. Ittyachan, P. Sagayaraj, J. Cryst. Growth 249 (2003) 557-560.
- [36] M.K. Marchewka, S. Debrus, A. Pietraszko, A.J. Barnes, H.J. Ratajczak, J. Mol. Struct. 656 (2003) 265–273.
- [37] J. Zyss, Molecular Nonlinear Optics: Materials, Physics and Devices, Academic, Boston, 1994.
- [38] K. Clays, B. Coe, J. Chem. Mater. 15 (2003) 642-648.
- [39] A. Ben Ahmed, H. Feki, Y. Abid, C. Minnot, Spectrochim. Acta A 75 (2010) 1315–1320.
- [40] M.G. Papadopoulos, A.J. Sadlej, J. Leszscynski, Non-Linear Optical Properties of Matter Publication Series Challenges and Advances in Computational Chemistry and Physics, vol. 1, Springer, Berlin, Germany, 2006.
- [41] S. Miertus, E. Scrocco, J. Tomassi, J. Chem. Phys. 55 (1981) 117.
- [42] R. Cammi, J. Tomasi, J. Comput. Chem. 16 (1995) 1449–1458.
- [43] J.B. West, J. Appl. Physiol. 87 (1999) 1543-1545.