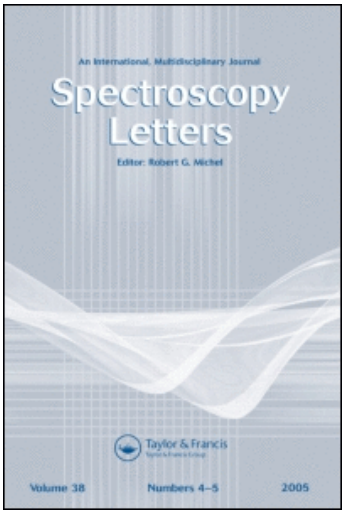


Spectroscopy Letters
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597299

Crystal Structure and Conformational Analysis of 4-[(*p-N,N*-Dimethylamino) benzylidene]-2-(3,5-dinitrophenyl)oxazole-5-one

Resul Sevinçek[a]; Gülsiye Öztürk[b]; Muhittin Aygün[a]; Mustafa Yavuz Ergün[b]; Serap Alp[b]; Orhan Büyükgüngör[c]
[a] Department of Physics, Faculty of Arts & Sciences, Dokuz Eylül University, Buca, İzmir, Turkey [b] Department of Chemistry, Faculty of Arts & Sciences, Dokuz Eylül University, Buca, İzmir, Turkey [c] Department of Physics, Faculty of Arts & Sciences, Ondokuz Mayıs University, Kurupelit, Samsun, Turkey

To cite this Article Sevinçek, Resul , Öztürk, Gülsiye , Aygün, Muhittin , Yavuz Ergün, Mustafa , Alp, Serap and Büyükgüngör, Orhan(2009) 'Crystal Structure and Conformational Analysis of 4-[(*p-N,N*-Dimethylamino) benzylidene]-2-(3,5-dinitrophenyl)oxazole-5-one', Spectroscopy Letters, 42: 1, 1 — 6
To link to this Article: DOI: 10.1080/00387010802428708
URL: http://dx.doi.org/10.1080/00387010802428708

Spectroscopy Letters, 42:1–6, 2009

ISSN: 0038-7010 print/1532-2289 online
DOI: 10.1080/00387010802428708

Taylor & Francis
Taylor & Francis Group

Crystal Structure and Conformational Analysis of 4-[(*p*-*N*,*N*-Dimethylamino) benzylidene]-2-(3,5-dinitrophenyl) oxazole-5-one

Resul Sevinçek[1], Gülsiye Öztürk[2], Muhittin Aygün[1], Mustafa Yavuz Ergün[2], Serap Alp[2], and Orhan Büyükgüngör[3]

[1]Department of Physics, Faculty of Arts & Sciences, Dokuz Eylül University, Buca, İzmir, Turkey
[2]Department of Chemistry, Faculty of Arts & Sciences, Dokuz Eylül University, Buca, İzmir, Turkey
[3]Department of Physics, Faculty of Arts & Sciences, Ondokuz Mayıs University, Kurupelit, Samsun, Turkey

ABSTRACT An azlactone derivative, 4-[(*p*-*N*,*N*-dimethylamino)benzylidene]-2-(3,5-dinitrophenyl)oxazol-5-one (DNPO), $C_{18}H_{14}N_4O_6$, has been synthesized, and its crystal structure has been investigated by single crystal X-ray analysis and *ab initio* method. DNPO is monoclinic, with $a = 9.3628(4)$ Å, $b = 13.5148(9)$ Å, $c = 13.7701(6)$ Å, $\beta = 92.921(4)^\circ$, $Z = 4$, $D_x = 1.46\,g/cm^3$, $\mu(MoK_\alpha) = 0.112\,mm^{-1}$, and space group P $12_1/c1$. The whole molecule is almost planar. The crystal structure is stabilized by C—H···N type intramolecular, C—H···O type intermolecular interactions. To determine the flexibility of DNPO, the selected torsion angle is varied from -180° to 180° in steps of 10°, and the molecular energy profile is calculated and analyzed.

KEYWORDS azlactones, conformational analysis, crystal structure

INTRODUCTION

5-Oxazolones are important intermediates for various organic syntheses, especially in the synthesis of [alpha]-keto and arylacetic acids, aminoacids, and peptides.[1,2] Azlactones give low fluorescence quantum yields. The fluorescence of the 5-oxazolone ring increases with substituted aryl groups, which already have emission characteristics.[3] Derivatives of 4-arylidene-2-aryl-oxazole-5-one have been studied as a precursor to some organic compounds, such as amino acids, amide-containing polymers,[4] and a wide range of biologically active compounds,[5] and also as a pH sensor and an alternative indicator for enzymatic glucose sensing.[6–8]

Here, we report the molecular and crystal structure of DNPO by single crystal X-ray diffraction study, and the conformational analysis with respect to a selected torsion angle is achieved by using 6-31G basis set at the Hartree–Fock level.

MATERIALS AND METHODS

UV-Vis absorption spectra were recorded with a Shimadzu (Tokyo, Japan) UV-1601 spectrophotometer. Fluorescence measurements were

Received 19 March, 2007; accepted 8 May, 2008.

Address correspondence to Muhittin Aygün, Department of Physics Facultiy of Arts & Science, Dokuz Eylül University, Buca, 35160 İzmir, Turkey. E-mail: muhittin.aygun@deu.edu.tr

performed by using a Varian-Cary Eclipse spectrofluorimeter (Ivarian, Molgrave, Australia). IR spectrum was recorded on a Perkin Elmer (Wellesley, MA) Spectrum BX FTIR spectrometer as KBr pellets. ^{1}H NMR spectra were recorded on a Varian Mercury AS 400 NMR spectrometer at 400 MHz.

Synthesis

A solution of *p-N,N*-dimethylaminobenzaldehyde (1 g, 6.7 mmol), 3,5-dinitrobenzoylglycine (1.8 g, 6.7 mmol), acetic anhydride (1.3 mL, 13.4 mmol), and sodium acetate (0.91 g, 6.7 mmol) was heated: after liquefaction, heating was continued for an additional 2 h. After the completion of the reaction (TLC analysis), 20 mL ethanol was added and the product (Scheme 1) kept at room temperature for 18 h. The solid product thus obtained was purified by washing with cold ethanol, hot water, and then a small amount of hexane. The solid was recrystallized from hot ethanol, and red crystals were obtained.

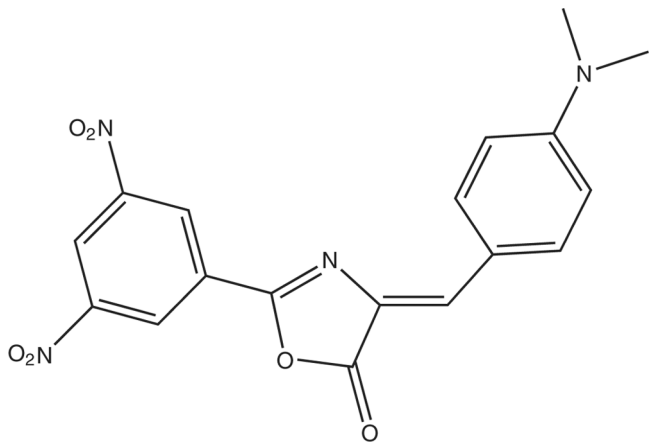
Spectroscopic Details

UV-Vis Absorption and Emission Spectra

DNPO dye exibited long wavelength absorption and emission maxima in solutions of dichloromethane (DCM), acetonitrile (ACN), and tetrahydrofuran (THF) (Table 1). In all of the employed solvents, the excitation wavelength was chosen as 500 nm and emission spectra were recorded.

IR Spectroscopy

FT-IR (KBr, cm^{-1}): 3091 (C−H, aromatic); 2861 (C−H, aliphatic); 1769 (C=O); 1641 (C=N); 1525, 1375, 1342 (NO_2); 1163 (C−O).



SCHEME 1 Chemical diagram of the title molecule.

TABLE 1 UV-Vis Absorption Maxima, λ_{max}^{abs}, and Emission Maxima, λ_{max}^{emis}, of the Title Molecule in Solvents of DCM, ACN, and THF

Solvent	λ_{max}^{abs} (nm)	λ_{max}^{emis} (nm)
DCM	518	558
ACN	503	584
THF	503	574

^{1}H NMR

^{1}H NMR of 2-(3,5-dinitrophenyl)-4-(3-*N,N*-dimethylaminophenylmethylene)-oxazol-5-one ($CDCl_3$, 400 MHz, δ (ppm)): 3.05–3.25 (s, 6H, $(CH_3)_2N-$); 6.72–6.85, 8.05–8.2 (d, d 2H, 2H $(CH_3)_2N-C-CH=CH-$, $(CH_3)_2N-C\underline{CH}=\underline{CH}-$); 7.32–7.40 (s, 1H, $=N-C_6H_4-\underline{CH}=$); 9.1–9.16 (s, 1H, $=C(NO_2)-CH=C(NO_2)-$); 9.17–9.26 (s, 2H, $=C(NO_2)-CH=C-C=N-$).

X-ray Crystallographic Details

A single crystal of size 0.58 × 0.38 × 0.23 mm was selected for the crystallographic study. All diffraction measurements were performed at room temperature (293 K) using graphite monochromated Mo-K_α radiation of wavelength 0.71073 Å and an STOE (Darmstadt, Germany) IPDS II diffractometer. Accurate cell parameters and orientation matrix were determined by least-squares refinement of the setting angles for 32,064 reflections collected in the range $2.11^\circ < \theta < 27.92^\circ$. The systematic absences and intensity symmetries indicated the monoclinic $P12_1/c1$ space group. Total 10,636 reflections with $\theta_{max} = 27.8^\circ$ ° were collected in the rotation mode. The intensities were corrected for Lorentz and polarization factors, but not for absorption effect ($\mu = 0.087\,mm^{-1}$).

The structure was solved by direct methods using SHELXS-97.[9] The structure was refined (on F^2) using full-matrix least-squares methods on the positional and anisotropic temperature parameters of the non-hydrogen atoms, and isotropic temperature parameters for H atoms. The structure was refined to $R = 0.046$ for the observed reflections and $R = 0.092$ for all data, Goof (Goodness of fit) $S = 0.953$ by using the intensity (I) values of 2304 reflections satisfying the $I > 2\sigma(I)$ criterion and 4042 reflections in refinement for 309 crystallographic parameters. The maximum peak and deepest hole observed in the Δρ map were 0.192 and −0.225 $eÅ^{-3}$, respectively.

TABLE 2 Crystallographic Data for the Title Compound

Color/shape	Red/prism
Chemical formula	$C_{18}H_{14}N_4O_6$
Formula weight	382.3
Temperature (K)	293(2)
Crystal system	Monoclinic
Space group	P $12_1/c1$
Unit cell dimensions	
a (Å)	9.3628(4)
b (Å)	13.5148(9)
c (Å)	13.7701(6)
β (°)	92.921(4)
Volume (Å^3)	1740.15(4)
Z	4
Density (calculated), (g/cm^3)	1.46
Absorption coefficient (mm^{-1})	0.112
Calculated T_{min}, T_{max}	0.945, 0.982
Diffractometer/meas. meth.	STOE IPDS II/rotation
Orange for data calculation (°)	2.7–27.8
Unique reflections measured	4042
Independent/observed reflections	4042/2340
Data/restraints/parameters	4042/0/309
Goodness of fit on F^2	0.953
Final R indices [$I > 4\sigma(I)$]	$R_1 = 0.046$, $wR_2 = 0.097$
R indices (all data)	$R_1 = 0.092$, $wR_2 = 0.111$

The scattering factors were taken from SHELXL-97.[9] The data collection conditions and parameters of refinement process are listed in Table 2.

Computational Details

The geometry optimization of the molecule leading to energy minima was achieved by using 6-31G[10] basis set at the restricted Hartree–Fock (RHF) level.[11] In order to determine the most stable conformation, the selected torsion angle T1 (N1–C9–C10–C11) is varied from –180° to 180° in 36 steps, and molecular energy profile is obtained by performing single point energy calculations on the calculated potential energy surface. All of the calculations were performed by using Gaussian 03 W.[12]

RESULTS AND DISCUSSION

An ORTEPIII diagram[13] with the atom numbering scheme with intramolecular weak interaction is shown in Fig. 1. The atomic coordinates and their equivalent isotropic thermal parameters are listed in Table 3. Comparative results obtained from X-ray crystallographic and computational studies are listed in Table 4.

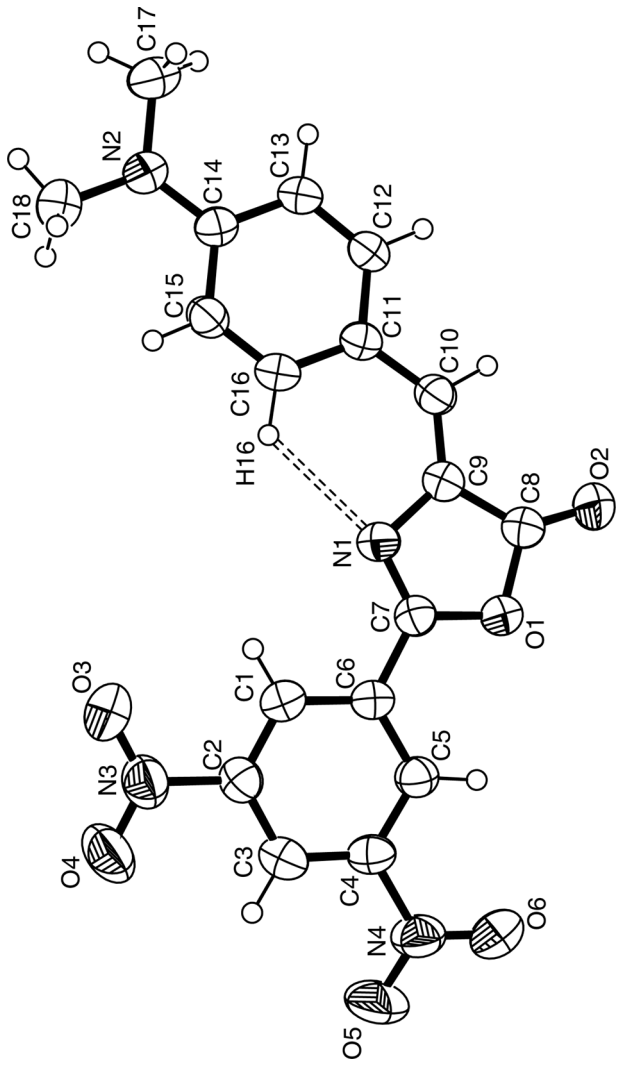


FIGURE 1 An ORTEP III view of the title molecule showing intra-molecular weak interactions with the atomic numbering of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level.

The bond distances and angles of the oxazolone ring are compared with these similar compounds,[14,15] especially, the N1–C9, C8–C9 single bonds and the double bond of the C7=N1; the O1–C8–O2 exocyclic bond angle, and C7–N1–C9, C7–O1–C8 bond angles; and N1–C9–C10–C11 torsion angle.

4-Arylidene-2-aryl-oxazole-5-one derivatives have planar geometry.[16,17] In agreement with the literature, DNPO also has planar geometry. The angle between C1...C6 and oxazolone ring planes is 2.66(13)°; and between C11...C16 and oxazolone ring planes is 1.97(13)°. The largest displacement from the mean plane of oxazolone ring is observed for C7 with a maximum deviation of 0.006(1) Å. Both

TABLE 3 Atomic Coordinates and Equivalent Isotropic Displacement Parameters. U_{eq} is Defined as One Third of the Trace of the Orthogonalized U_{ij} tensor

Atom	x (Å)	y (Å)	z (Å)	U_{eq} (Å^2)
O1	0.5694(1)	0.7239(1)	0.4229(1)	0.0523(3)
O2	0.6865(2)	0.7299(1)	0.2826(1)	0.0705(5)
O3	0.4999(3)	0.4864(2)	0.8126(1)	0.1090(8)
O4	0.3536(2)	0.5760(1)	0.8887(1)	0.0881(6)
O5	0.1781(3)	0.8806(2)	0.7470(1)	0.1076(7)
O6	0.2071(2)	0.9077(1)	0.5966(1)	0.0791(5)
N1	0.6578(2)	0.5824(1)	0.4897(1)	0.0437(4)
N2	1.0979(2)	0.1910(1)	0.4974(1)	0.0564(4)
N3	0.4255(2)	0.5591(2)	0.8197(1)	0.0647(5)
N4	0.2303(2)	0.8608(1)	0.6705(1)	0.0636(5)
C1	0.4973(2)	0.6111(2)	0.6589(1)	0.0456(4)
C2	0.4182(2)	0.6295(1)	0.7379(1)	0.0465(4)
C3	0.3314(2)	0.7114(2)	0.7445(1)	0.0501(5)
C4	0.3251(2)	0.7749(1)	0.6668(1)	0.0471(4)
C5	0.4028(2)	0.7606(1)	0.5854(1)	0.0453(4)
C6	0.4892(2)	0.6777(1)	0.5813(1)	0.0412(4)
C7	0.5748(2)	0.6569(1)	0.4981(1)	0.0432(4)
C8	0.6666(2)	0.6871(2)	0.3564(1)	0.0506(5)
C9	0.7218(2)	0.5959(1)	0.4009(1)	0.0433(4)
C10	0.8232(2)	0.5387(1)	0.3618(1)	0.0438(4)
C11	0.8889(2)	0.4498(1)	0.3982(1)	0.0409(4)
C12	0.9913(2)	0.4024(1)	0.3437(1)	0.0455(4)
C13	1.0589(2)	0.3169(2)	0.3738(1)	0.0472(4)
C14	1.0288(2)	0.2739(1)	0.4638(1)	0.0429(4)
C15	0.9267(2)	0.3216(1)	0.5191(1)	0.0461(4)
C16	0.8595(2)	0.4064(1)	0.4877(1)	0.0442(4)
C17	1.1872(3)	0.1331(2)	0.4363(2)	0.0671(6)
C18	1.0541(4)	0.1428(2)	0.5856(2)	0.0698(7)

six-membered rings are nearly planar with a maximum deviation of 0.006(1) Å.

Besides the van der Waals interactions, the crystal structure is stabilized by C–H···N type intramolecular and C−H···O type intermolecular weak interactions, of which details are given in Table 5, and Pluton[18] molecular packing drawing with intermolecular weak interactions in the unit cell of DNPO is shown in Fig. 2. The one-dimensional assemblies formed by hydrogen bonding are enforced by weaker intermolecular interactions. C13 in the molecule at (x,y,z) acts as a hydrogen-bond donor, via H13, to atom O2 in the molecule $(2-x, 1/2+y, -1/2-z)$, while atom C13 at $(2-x, 1/2+y, -1/2-z)$, in turns, acts as donor to O2 at (x, 1 + y, z). In this manner, a C(8)[19] chain is formed, running along the b-axis. In a similar fashion, C5 in the molecule at (x,y,z) acts as a hydrogen-bond donor, via H5, to atom O4 in the molecule $(x, -1/2-y, 1/2+z)$, and atom C5 at $(x, -1/2-y, 1/2+z)$, in turns, acts as donor to O4 at (x, y, 1 + z). In this manner, a C(7)[19] chain is formed, running along the c-axis.

There are two π–π stacking interactions relating to the R1 (C1...C6) ring [fractional centroid coordinates: 0.41067(8), −0.19419(6), 0.16247(5), Cg(1)] and R2 (C11...C16) ring [fractional coordinates: 0.95902(8), 0.13815(6), −0.06896(5), Cg(2)] in the crystal structure. R1 at (x, y, z) interacts with R2 at $(1-x, -y, -z)$; in the same manner, R2 at (x, y, z) interacts with R1 at $(1-x, -y, -z)$, so there forms a π–π interaction dimer. The perpendicular distances of these π–π stacking interactions (R1–R2) are found to be 3.709(1) Å.

TABLE 4 Selected Bond Distances (Å), Bond Angles (°), and Torsion Angles (°)

	X-ray	*Ab initio*
Bond distances		
O(1)–C(7)	1.374(2)	1.381
O(1)–C(8)	1.413(2)	1.405
O(2)–C(8)	1.191(2)	1.200
N(1)–C(7)	1.281(2)	1.270
N(1)–C(9)	1.401(2)	1.416
C(6)–C(7)	1.459(2)	1.454
C(9)–C(10)	1.357(3)	1.344
C(10)–C(11)	1.428(3)	1.441
Bond angles		
C(7)–O(1)–C(8)	104.9(1)	107.11
C(7)–N(1)–C(9)	105.3(1)	107.22
C(1)–C(6)–C(7)	117.8(1)	119.38
O(1)–C(7)–N(1)	116.7(2)	114.22
O(2)–C(8)–C(9)	134.4(2)	133.45
N(1)–C(9)–C(8)	108.6(2)	107.57
N(1)–C(9)–C(10)	127.7(2)	128.65
Torsion angles		
C(7)−O(1)−C(8)−O(2)	179.7(2)	−179.99
C(1)−C(6)−C(7)−N(1)	0.1(3)	0.00
N(1)−C(9)−C(10)−C(11)	−1.6(3)	0.00
C(9)−C(10)−C(11)−C(12)	−179.2(2)	180.00

TABLE 5 Details Related to Both Intermolecular and Intramolecular Weak Interactions (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
C(16)–H(16)···N(1)	0.99(2)	2.36(2)	3.038(2)	124.8(13)
C(13)–H(13)···O(2)^{i}	0.97(2)	2.54(2)	3.497(2)	171.8(16)
C(5)–H(5)···O(4)^{ii}	0.94(2)	2.57(2)	3.507(3)	175.6(19)

Note: D, donor, A, acceptor. Symmetry transformation used to generate the equivalent atoms. Symmetry codes: i: $2-x, 1/2+y, -1/2-z$; ii: $x, -1/2-y, 1/2+z$.

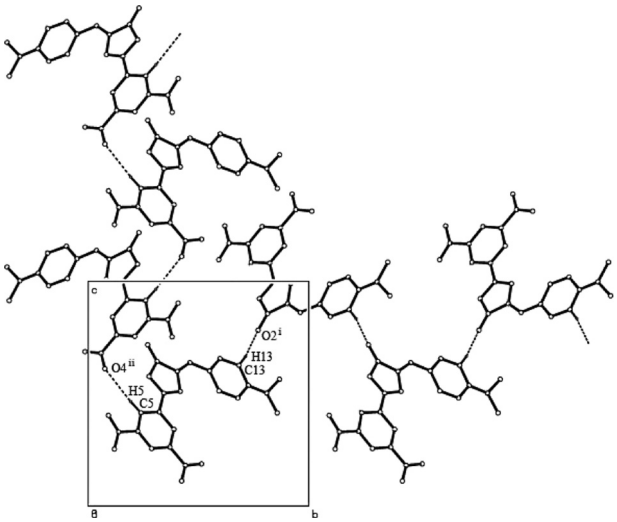


FIGURE 2 **Unit-cell contents with the inter-molecular hydrogen-bonding scheme indicated by dashed lines, viewed along the a-axis. Symmetry codes: i: 2 – x,1/2 + y, – 1/2 – z; ii: x, – 1/2 – y, 1/2 + z.**

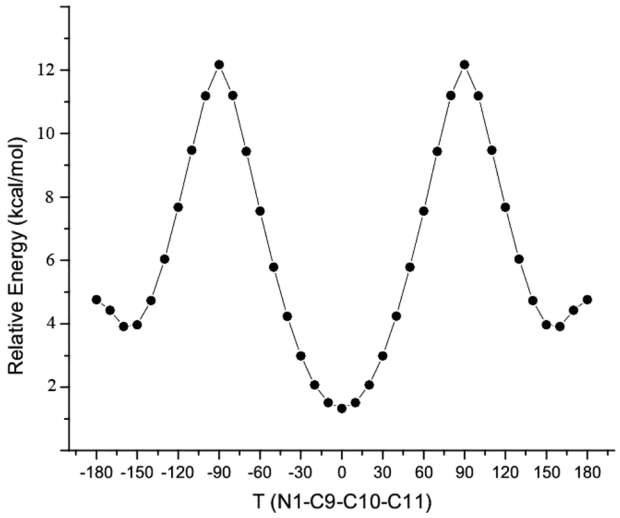


FIGURE 3 **Variation of the heat of formation versus selected torsion angle.**

In order to obtain the most stable conformation of DNPO, the torsion angle T (N1–C9–C10–C11) was chosen because it determines the isomerism (*E* or *Z*). According to crystallographic study, T is obtained as $-1.6(3)^\circ$, whereas this torsion angle is 0.0° in the optimized molecular structure corresponding with the most stable pseudo-conformer. *Ab initio* methods cannot represent the structural properties of the crystalline materials comprehensively, because they have some foibles such regarding as a single molecule throughout the computations. For these reasons, some discrepancies are observed between the molecular conformations of the optimized structure and the X-ray structure. The observed conformational difference in optimized structure is presumably due to weak intermolecular and intramolecular hydrogen bonding and the contribution from packing of the molecules obeyed space group symmetry operations. The *ab initio* molecular orbital calculations were carried out in order to define the conformational flexibility of DNPO as a function of the torsion angle T. Variation of heat of formation against the torsion angle T is shown in Fig. 3. The energy profile as a function of T has two nearly global maxima in the vicinity of -90° and 90°. The energy profile has a minimum in the vicinity of 0°. When T is 0°, the molecule is in Z isomerism. There are two local minima in the vicinity of -160° and 160°; the molecule is nearly in *E* isomerism. According to the conformational analysis, the most stable conformation of DNPO is in *Z* isomerism, in agreement with the X-ray crystallographic results.

ACKNOWLEDGMENTS

The authors thank Dokuz Eylül University Research Fund (project number 2007.KB.FEN.36) for financial support of this work. In addition, R.S. thanks TÜBİTAK (The Scientific and Technical Research Council of Turkey) for partial financial support.

REFERENCES

1. Leplawy, M. T.; Jones, D. S.; Kenner, G. W.; Sheppard, R. C. Peptides—XI: Synthesis of peptides derived from alpha-methylalanine. *Tetrahedron* **1960**, *11*, 39–51.
2. Lechmann, J.; Linden, A.; Heimgartner, H. Site-selective incorporation of thioamide-linkages into a growing peptide. *Tetrahedron* **1999**, *55*, 5359–5376.
3. İçli, S.; Icil, H; Alp,S.; Koç, H. NMR, absorption and fluorescence parameters of azlactones. *Spectrosc. Lett.* **1994**, *27*(9), 1115–1128.
4. Reed, J. W.; Kingston, G. I. D. Biosynthesis of antibiotics of the virginiamycin family, 5. The conversion of phenylalanine to phenylglycine in the biosynthesis of virginiamycin S1. *J. Nat. Prod.* **1986**, *49*, 629.
5. Bacse, H. J.; Havsteen, B. Oxazolones as substrates in active site titrations of hydrolases. *Anal. Biochem.* **1989**, *181*, 321.
6. Ertekin, K.; Alp, S.; Karapire, C.; Yenigül, B.; Hendena, E.; İçli, S. Fluorescence emission studies of an azlactone derivative embedded in polymer films. An optical sensor for pH measurements. *J. Photochem. and Photobiol. A.* **2000**, *137*, 155–161.
7. Ertekin, K.; Çinar, S.; Aydemir, T.; Alp, S. Glucose sensing employing fuorescent pH indicator: 4-[(p-N,N-dimethylamino)benzylidene]-2-phenyloxazole-5-one. *Dyes Pigments* **2005**, *67*, 133–138.
8. Ertekin, K.; Karapire, C.; Alp, S.; Yenigül, B.; İçli, S. Photophysical and photochemical characteristics of an azlactone dye in sol-gel matrix; a new fluorescent pH indicator. *Dyes Pigments* **2003**, *56*, 125–133.
9. Sheldrick, G. M. SHELXS-97 and SHELXL-97. University of Göttingen: Göttingen, Germany **1997**.

10. Hehre, W. J.; Ditchfield, R.; Pople, J. A.; Self-consistent molecular orbital methods. XII. Further extensions of Gaussian-type basis sets for use in molecular orbital studies of organic molecules. *J. Chem. Phys.* **1972**, *56*, 2257–2261.
11. Roothan, C. C. J. New developments in molecular orbital theory. *Rev. Mod. Phys.* **1951**, *23*, 69–89.
12. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr., T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 03, Revision B.05. Gaussian, Inc.: Pittsburgh, PA, 2003.
13. Farrugia, L. J. ORTEP-3 for Windows—a version of ORTEP-III with a graphical user interface (GUI). *J. Appl. Cryst.* **1997**, *30*, 565.
14. Vasuki, G.; Parthasarathi, V.; Ramamurthi, K.; Singh R. M.; Srivastava A. 2-Phenyl-4-(p-toluidinomethylene)-5-oxazolone. *Acta Cryst.* **2001**, *E57*, o120–o121.
15. Wang, X.; Zhang, M.; Qi, Z.; Ma, S. 2-Methoxy-4-[2-methyl-5-oxo-4,5-dihydro-1,3-oxazol-4-ylidene)methyl]phenyl acetate. *Acta Cryst.* **2005**, *E61*, o1265–o1266.
16. Sun, Y.; Wang, X.; Li, J.; Zheng, Z.; Wu R. 2,6-Dimethoxy-4-(5-oxo-2-phenyl-4,5-dihydro-1,3-oxazol-4-ylidenemethyl)-phenyl acetate. *Acta Cryst.* **2007**, *E63*, o4426.
17. Şen, B.; Öztürk, G.; Alp, S.; Aygün, M.; Büyükgüngör, O. 2-Methoxy-4-[(5-oxo-2-phenyl-4,5-dihydro-1,3-oxazol-4-ylidene)methyl]-phenyl 4-methylbenzenesulfonate. *Acta Cryst.* **2007**, *C63*, o223-o224.
18. Spek, A. L. Single-crystal structure validation with the program. *J. Appl. Cryst.* **2003**, *36*, 7–13
19. Bernstein, J.; Davis, R. E.; Shimoni, L.; Chang, N.-L. Patterns in Hydrogen Bonding: Functionality and Graph Set Analysis in Crystals. *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 1555–1573.