



Research Article

Synthesis, molecular structure, spectroscopic and computational studies of (*E*)-*tert*-butyl (2-((3,5-di-*tert*-butyl-2-hydroxybenzylidene) amino)ethyl) carbamate as a functionalized schiff base

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ABSTRACT**Keywords:**

Synthesis,
crystal structure,
schiff base,
amine,
mono-Boc-protection,
theoretical calculation

This work presents the synthesis and characterization of a novel compound, (*E*)-*tert*-butyl (2-((3,5-di-*tert*-butyl-2-hydroxybenzylidene)amino)ethyl)carbamate as the Schiff base derivative. This compound has been designed as an unsymmetrical ligand. The spectroscopic properties of the compound were examined by FT-IR, ¹H NMR, ¹³C NMR, MS and elemental analyses. The molecular structure of the compound was also confirmed using X-ray single-crystal data. The molecule is stabilized through intermolecular N—H···O hydrogen bonds, which form chains extending along [100]. And also it has been calculated; molecular structure, vibrational frequencies and ¹H and ¹³C NMR chemical shifts of the title compound by using B3LYP method with 6-311++G(dp) basis set, as well.

TR

Fonksiyonelleştirilmiş schiff bazı olarak (*E*)-*tert*-butil (2-((3,5-di-*tert*-butil-2-hidroksibenziliden)amino)etil)karbamat'ın sentezi, moleküler yapı, spektroskopik ve hesaplamalı çalışmaları

Ö Z E T**Anahtar Kelimeler:**

Sentez,
Kristal yapı,
Schiff bazı,
amin,
monoBoc koruma,
teorik hesaplama

Bu çalışma, Schiff baz türevi olarak yeni bir bileşiğin, (*E*)-*tert*-butil (2-((3,5-di-*tert*-butil-2-hidroksibenziliden) amino) etil) karbamat'ın sentezini ve karakterizasyonunu içermektedir. Bu bileşik, simetrik olmayan katalizör olarak potansiyel bir aday olan simetrik olmayan metal komplekslerinin hazırlanması için bir ligand olarak seçilmiştir. Bileşiğin spektroskopik özellikleri FT-IR, ¹H NMR, ¹³C NMR, kütle ve element analizleriyle incelenmiştir. Bileşiğin moleküler yapısı, ayrıca X-ışını tek kristalli verileri kullanılarak doğrulanmıştır. Molekül, (100) boyunca uzanan zincirleri oluşturan moleküller arası N-H···O hidrojen bağları ile stabilize edilir. Ayrıca bileşiğin, moleküler yapı, titreşim frekansları ve ¹H ve ¹³C NMR kimyasal kaymaları, B3LYP yöntemi kullanılarak 6-311 ++ G (dp) temel seti ile hesaplanmıştır.

1. Introduction

Schiff bases are multipurpose ligands synthesized from the condensation of an amino compound with carbonyl compounds and these coordinate to metal ions via azomethine nitrogen and have been studied extensively [1, 2]. They have wide applications in analytical chemistry and in medicine. The C=N linkage is essential in biological processes including antifungal, antibacterial and anticancer activities [3, 4].

Moreover, the use of Schiff bases as a fluorescent sensor sensitive to metal ions is a promising research area in chemistry and has a profound role in ecological, biological and clinical applications [5, 6].

Schiff base ligands also played an important role in the development of coordination chemistry because of forming complexes with most transition metals [7]. The complexes of Schiff bases which exhibit interesting physical, chemical and biological properties have broad range of utilization in various areas of science such as in agriculture, pharmaceutical and industrial chemistry [8,9]. In this study, we designed a new type of Schiff base with the reaction of an aromatic aldehyde and ethylenediamine derivative carrying terminal Boc-protective group to obtain (*E*)-*tert*-butyl (2-((3,5-di-*tert*-butyl-2-hydroxybenzylidene)amino)ethyl)carbamate (**3**). This Schiff base can be used for the preparation of unsymmetrical metal complexes for further studies.

By the deprotection of the amine end of **3** and the reaction of different aldehyde derivative. We performed the synthesis, characterization and the crystal structure of the compound **1** as well as the experimental and theoretical.

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2. Experimental

2.1. Chemicals and instruments

The following chemicals were obtained from Sigma-Aldrich; 2,4-ditert-butylphenol, urotropin, glacial acetic acid, ethylenediamine, di-tert-butyl dicarbonate, dichloromethane (DCM), chloroform (CHCl₃), hexane, diethylether, methanol (MeOH), ethanol (EtOH). All other reagents and solvents were reagent grade quality and obtained from commercial suppliers. All solvents were stored over molecular sieves (4Å) after they dried and purified as described by Perrin and Armarego [10]. Oxygen free inert atmosphere was supplied by argon through dual-bank vacuum-gas manifold system. Thin-Layer chromatography (TLC) was performed using silica gel 60-HF254 as an adsorbent. Column chromatography was performed with silica gel (Merck grade 60) and the size exclusion chromatography with Bio-beads gel (SX-1.) Infrared spectra were recorded on a Perkin Elmer Spectrum two FT-IR spectrophotometer equipped with Perkin Elmer UATR-TWO diamond ATR and corrected by applying the atr-correction function of Perkin Elmer Spectrum software. ¹H and ¹³C NMR spectra were recorded a Varian Mercury Plus 300 MHz spectrometer. Electrospray ionization mass spectrum measurement was obtained on an Agilent 6230 A LC-TOF/MS Spectrometer in positive mode. The elemental compositions of the samples were analyzed by an element analyzer (Flash 2000, Thermo Scientific).

2.2. Computational Details

The molecular structure of (*E*)-tert-butyl (2-((3,5-di-tert-butyl-2-hydroxybenzylidene) amino)ethyl)carbamate in the ground state (in vacuo) is computed by performing the density functional theory (DFT) by a hybrid functional B3LYP functional (Becke's three parameter hybrid functional using the LYP correlation functional) methods [11,12] at 6-311++G(d,p) level. The optimized geometrical structure, IR and NMR spectra were calculated by using Gaussian 09W program package [13] and the obtained results were visualized by Gauss-View 5 program [14]. ¹H and ¹³C NMR chemical shifts of the title compound were calculated within the gauge-independent atomic orbital (GIAO) approach [15,16] which is one of the most common approaches for calculating nuclear magnetic shielding tensors. Additionally, harmonic vibrational frequencies for the title compound calculated by B3LYP level in conjunction with 6-311++G(d,p) basis set were scaled down by 0.96 in order to improve well-known errors such as anharmonicity and basis set deficiencies.

2.3. X-ray crystallography

The single X-ray diffraction data were obtained using the STOE IPDS II diffractometer equipped with graphite filter. The crystal data together with the refinement details for the compound are included in Table 1. Unit cell parameters of the compound were determined by using WinGX software [17]. The structure of the titled compound was solved by the direct methods procedure in SHELXS-97 program [18] and all the non-hydrogen atoms were refined anisotropically using the SHELXL-2014/7 program [19]. The molecular figures are prepared with the help of Mercury and ORTEP-3 program packages [20,21]. All geometrical calculations were carried out using the program PLATON [22]. All the non-hydrogen atoms were fixed geometrically. The hydrogen atoms were placed in calculated positions with C—H = 0.82–0.97 Å and refined using a riding model with U_{iso}(H₃) = 1.5U_{eq}(O₃) for hydroxybenzylidene ring's oxygen atom and U_{iso}(H) = 1.2U_{eq}(C, N, O) for the other groups.

CCDC 1830725 contains supplementary crystallographic data (excluding structure factors) for the compound reported in this article. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/deposit> [or from the Cambridge Crystallographic Data Center (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223 336033; e-mail: deposit@ccdc.cam.ac.uk].

Table 1. Crystallographic data and refinement parameters for the compound, C₂₂H₃₆N₂O₃

Crystal data	
Chemical formula	C ₂₂ H ₃₆ N ₂ O ₃
Mr	376.53
Crystal system, space group	Monoclinic, P2 ₁ /c
Temperature (K)	296
a, b, c (Å)	13.184 (2), 19.1485 (19), 9.2696 (13)
β (°)	95.123 (13)
V (Å ³)	2330.8 (6)
Z	4
Radiation type	Mo Kα
μ (mm ⁻¹)	0.07
Crystal size (mm)	0.50 × 0.283 × 0.120
Data collection	
Diffractometer	STOE IPDS 2 diffractometer
Absorption correction	Integration
Tmin, Tmax	0.9762, 0.9929
No. of measured, independent and observed [I > 2σ(I)] reflections	19690, 4118, 1764
Rint	0.115
(sin θ/λ)max (Å ⁻¹)	0.596
Refinement	
R[F ² > 2σ(F ²)], wR(F ²), S	0.098, 0.328, 1.03
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.48, -0.26

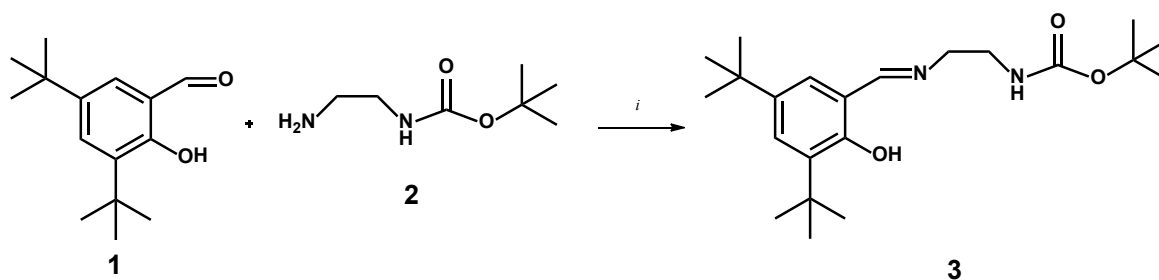
2.4. Synthesis

2.4.1. 3,5-di-tert-butyl-2-hydroxybenzaldehyde (1) and tert-butyl (2-aminoethyl)carbamate (2)

The preparation of **1** was carried out by the reaction of 2,4-ditert-butylphenol and urotropin in glacial acetic acid according to the published literature resulting in 94% yield [23]. Tert-butyl (2-aminoethyl)carbamate (**2**) has been obtained by reaction of ethylenediamine and di-tert-butyl dicarbonate at 0°C by applying the literature [24]. The obtained spectroscopic data are accordance with the literatures.

2.4.2. (*E*)-tert-butyl (2-((3,5-di-tert-butyl-2-hydroxybenzylidene) amino)ethyl)carbamate (3)

A solution of tert-butyl (2-aminoethyl)carbamate (**2**) (342 mg, 2.13 mmol) in dry EtOH (15 mL) was added to a solution of 3,5-di-tert-butyl-2-hydroxybenzaldehyde (**1**) (500 mg, 2.13 mmol) in EtOH (15 mL) and the mixture was heated up to 80°C for 12h. The progress of the reaction was monitored by TLC using (THF/Hegzan: 3/4) solvent system. When the reaction was completed, the reaction mixture was cooled to room temperature. The solvent was evaporated to 1/3 of the initial volume of the reaction mixture. The precipitated Schiff base (**3**) was filtered and washed successively with cold ethanol. The pale yellow solid obtained was recrystallized from hot ethanol to give the desired product in 85% yield. FT-IR (UATR-TWO™) ν_{max}/cm⁻¹: 3420 (NH), 3348 (OH), 3051 (Ar, C-H), 2956-2869 (Aliph., C-H), 1693 (C=O), 1631 (C=N), 1505 (C=C), 1468-1363 (C-C), 1272, 1250, 1170, 772. ¹H-NMR (DMSO) δ (ppm) : 13.88 (s, 1H, OH), 8.44 (s, 1H, C=N), 7.26 (d, 1H, ArH), 7.22 (s, 1H, ArH), 6.96 (t, 1H, NH), 3.59-3.55 (t, 2H, AliphH), 3.23-3.19 (t, 2H, AliphH), 1.34 (s, 9H, AliphH), 1.30 (s, 9H, AliphH), 1.23 (s, 9H, AliphH). ¹³C-NMR (DMSO) δ (ppm) : 168.80, 158.47, 156.41, 140.28, 136.48, 127.01, 126.71, 118.39, 78.32, 58.47, 35.21, 34.49, 31.97, 29.88, 28.84. MS (ESI-TOF): m/z 377.2775 [M+H]⁺. Anal. Calc. for C₂₂H₃₆N₂O₃(%): C, 70.18; H, 9.64; N, 7.44; O, 12.75; Found (%): C, 69.96; H, 9.66; N, 7.40.



Scheme 1. Synthesis route: (i) EtOH, 80°C, 12h

3. Results and Discussion

3.1. Synthesis and spectroscopic characterization

Scheme 1 shows the synthetic route for the target compounds **3**.

As a first step, 3,5-di-tert-butyl-2-hydroxybenzaldehyde (**1**) was prepared by reacting of commercially available 2,4-di-tert-butylphenol with urotropin in glacial acetic acid resulting in 94% yield using the literature procedure [23]. The other starting material, compound **2**, was obtained by the reaction of ethylenediamine and di-tert-butyl dicarbonate in dichloromethane by maintaining at 0°C during addition and then further stirring at room temperature for 24 hours by applying the literature [24].

The preparation of required Schiff base (**3**) was carried out in ethanol at reflux temperature by using corresponding aldehyde derivative (**1**) and tert-butyl (2-aminoethyl)carbamate (**2**) with 85% yield. Suitable crystal of the molecule (**3**) for X-ray analysis was obtained upon crystallization from hot ethanol solution.

Characterization of the target product (**3**) was carried out a combination of methods including FT-IR, ¹H-NMR, ¹³C-NMR, mass spectroscopy and elemental analysis. All the spectral data are in accordance with the proposed structures.

In the FT-IR spectra of **3**, formation of Schiff base treated with tert-butyl (2-aminoethyl)carbamate (**2**) to give compound **3** was confirmed by the disappearance of the band at 1645 cm⁻¹ (that band calculated at: 1701 cm⁻¹) belonging to the C=O stretching vibration of aldehyde group of **1** and appearance of C=N stretching vibration band at 1631cm⁻¹ and this band was calculated at: 1664 cm⁻¹, C=O stretching vibration band of Boc-group at 1631cm⁻¹. The calculated vibration bands of compound **3** are given in Table 2.

The ¹H-NMR data gave satisfactory information about the proposed structure of the target compound (**3**).

When compared the ¹H-NMR spectra of compound **1** and **3**, the disappearances of HC=O proton signal of 3,5-di-tert-butyl-2-hydroxybenzaldehyde (**1**) and the appearance of new peaks in aromatic region at 8.44 ppm belongs to the imine proton and the -NH

Table 2. Experimental and theoretical vibrational wavenumbers (cm⁻¹) for the title molecule

Assignments	FT-IR	Scaled wavenumbers	Unscaled wavenumbers
ν NH	3420	3496	3642
ν OH	3348	3723	3878
ν CH _(Ar.)	3051	3085	3214
ν CH _(Aliph.)	2956-2869	3013-2851	3139-2970
ν C=O	1693	1693	1764
ν C=N	1631	1630	1698
ν C=C	1505	1562	1627
ν C-C	1468-1363	1465-1359	1526-1416
β CH _(Aliph.)	1272	1270	1323
β CH _(Ar.)	1250	1246	1298
ν C-O	1170	1140	1188
γ CH _(Aliph.)	772	773	805

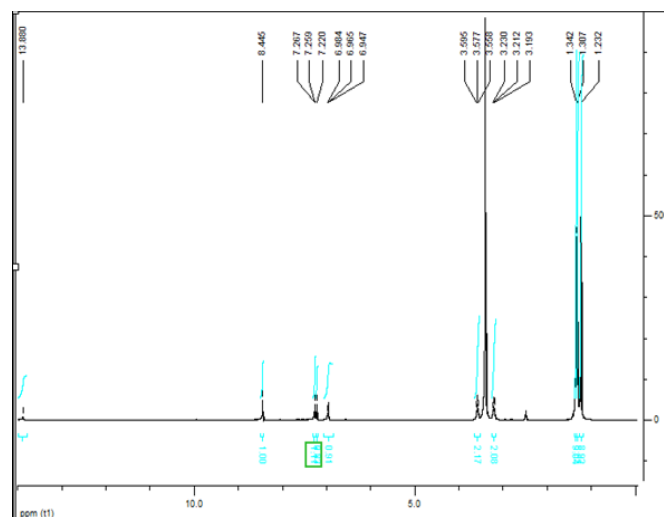


Fig.1. The ¹H NMR spectrum of **3**

peak at 6.96 ppm were the evidence of the formation of Schiff base derivative (**3**) and -NH peak was calculated at: 7.31ppm. In addition, tert-butyl peaks originating from the boc-protecting group were observed at 1.34 ppm as singlet and this peak was calculated at 1.41 ppm (Figure 1).

In the ¹³C-NMR spectrum of **3** the presence of the signals at 168.80 ppm and 158.47 ppm attributed to the imine and carbonyl atoms are the obvious differences from **1**. These signals were calculated at: 147.28 ppm and 162.78 ppm. For the ¹³C-NMR spectrum of **3**, the other characteristic signals were observed in the range of 78.32 ppm and 28.84 ppm related to tert-butyl carbons of boc-protecting group and these peak were calculated at: 28.76 ppm and 72.34 ppm. Also carbon peaks of CH₂ observed at 58.47 ppm and 35.21 ppm and these peaks were calculated at: 62.02 ppm and 39.78 ppm respectively (Figure 2).

The Mass spectrum of **3** was obtained by the Electrospray ionization mass spectrum confirming the proposed structures. In the mass spectrum of **3**, the presence of molecular ion peaks observed at high intensity and easily identified at m/z: 377.2775 [M⁺]⁺ clearly indicates the formation of desired product as seen in Fig. 3.

3.2. Crystal Structure Description of the Compound:

Structure crystallizes in the monoclinic space group P21/c with the cell parameters: a = 13.184 (2) Å, b = 19.1485 (19) Å, c = 9.2696 (13) Å, β = 92.26(3)°. Fig. 4 displays the structural formula with the numbering used in the crystallographic study. The selected bond lengths and angles and torsion angles for the titled compound are also presented in Table 3.

The molecule adopted an E configuration about the central C8=N2 double bond and for the dihedral angle between the mean planes of the hydroxybenzylidene ring and the C7/C6/N1/C5/O2 group was 57.3 (1)°. In carbamate group, O1—C5, O2—C5 and N1—C5 bond lengths are 1.351 (6) Å, 1.214 (6) Å and 1.344 (6) Å. These bond lengths were calculated: 1.359, 1.215 and 1.344 Å respectively. From

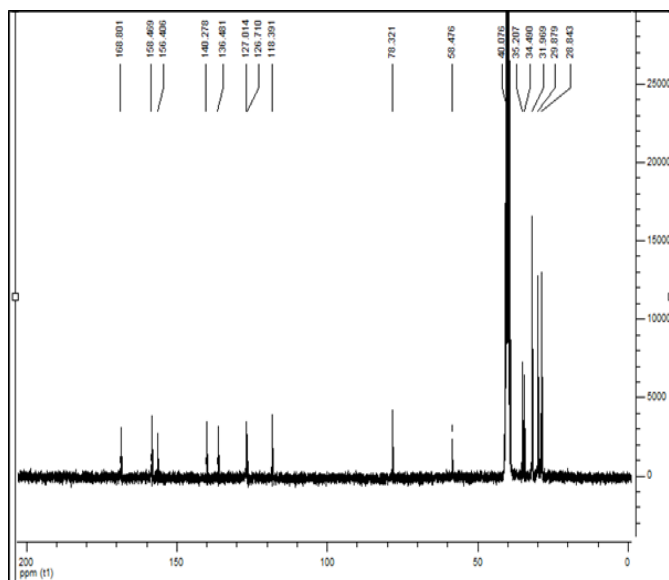


Fig. 2. The ^{13}C -NMR spectrum of **3**

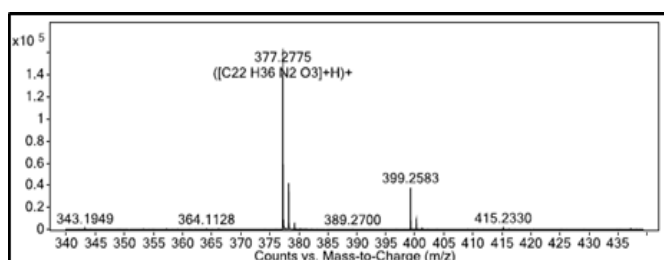


Fig. 3. Mass spectrum of **3**

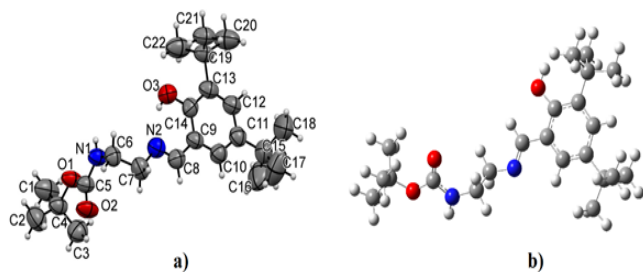


Fig. 4. a-b) The molecular structure of the title compound, showing the atom-numbering scheme and 30% probability displacement ellipsoids of non-hydrogen atoms. Optimized molecular structure (with B3LYP/6-311++G(d,p) level) of the title compound.

these results, all the bond lengths are with small deviation due to the hydrogen bond interactions. This is in agreement with the reported values [25,26] of the bond lengths of similar carbamate compounds. The mean plane of the carbamate $\text{N}-\text{C}(\text{O})-\text{O}$ group is twisted slightly from the attached butyl and $(\text{C}6-\text{C}7-\text{N}2-\text{C}8)$ groups, making respectively dihedral angles of $87.6(2)^\circ$ and $77.1(2)^\circ$ in this compound.

In the crystal, hydrogen-bonding is the dominant interactions. The molecule shows a near-planar V-shaped conformation, according to $\text{C}6-\text{C}7$ bond, which is stabilized by three intramolecular $\text{O}3-\text{H}3\cdots\text{N}2$, $\text{C}3-\text{H}3\text{C}\cdots\text{O}2$ and $\text{C}2-\text{H}2\text{B}\cdots\text{O}2$ hydrogen bonds (Fig.4 (a) and Table 4). These intramolecular hydrogen bond interactions (Fig. 5 (a)) exist forming a three pseudo-six-membered ring of $\text{N}(6)$ graph-set motifs. This contribution comes from the $\text{O}-\text{H}$ group on the phenyl ring and $\text{O}2$ atom of carbamate group. Also, the primary intermolecular hydrogen bond in the compound as $\text{N}1-\text{H}1\cdots\text{O}2^i$ is classed as strong/moderated classical hydrogen bonds with donor-acceptor ($\text{D}\cdots\text{A}$) distances $< 2.95 \text{ \AA}$ and $\text{D}-\text{H}\cdots\text{A}$ angles close to

linearity at 180° (Table 3). This hydrogen bond links the molecules to form chains, propagating along the (100) direction. The detailed all geometric parameters of hydrogen bonds are given in Table 3. Fig. 5 (b) depicts a view of the packing of the molecule in the unit cell, according to $\text{N}1-\text{H}1\cdots\text{O}2$ intermolecular hydrogen bond (green dashed line).

Table 3. Hydrogen-bond geometries (\AA , $^\circ$) for the titled compound

Bond lengths (\AA)	(Exp.)	(Theoretical)		(Exp.)	(Theoretical)
$\text{O}1-\text{C}5$	1.351	1.359	$\text{N}2-\text{C}7$	1.468	1.450
$\text{O}1-\text{C}4$	1.474	1.474	$\text{N}1-\text{C}5$	1.344	1.364
$\text{O}3-\text{C}14$	1.357	1.373	$\text{N}1-\text{C}6$	1.435	1.274
$\text{N}2-\text{C}8$	1.256	1.274	$\text{O}2-\text{C}5$	1.214	1.215
Bond angles ($^\circ$)					
$\text{C}5-\text{O}1-\text{C}4$	120.5	121.4	$\text{O}2-\text{C}5-\text{N}1$	124.3	124.7
$\text{C}5-\text{N}1-\text{C}6$	120.9	122.6	$\text{O}2-\text{C}5-\text{O}1$	125.6	125.9
$\text{C}8-\text{N}2-\text{C}7$	118.9	117.9	$\text{N}1-\text{C}5-\text{O}1$	110.1	109.5
$\text{N}2-\text{C}7-\text{C}6$	111.4	122.4	$\text{O}3-\text{C}14-\text{C}13$	120.5	122.3
$\text{O}1-\text{C}4-\text{C}1$	102.7	102.5	$\text{O}3-\text{C}14-\text{C}9$	118.3	115.6
$\text{O}1-\text{C}4-\text{C}3$	110.3	110.1	$\text{N}2-\text{C}8-\text{C}9$	123.6	122.4
Torsion angles ($^\circ$)					
$\text{C}6-\text{N}1-\text{C}5-\text{O}2$	-1.4	-2.1	$\text{C}4-\text{O}1-\text{C}5-\text{N}1$	176.7	178.5
$\text{C}6-\text{N}1-\text{C}5-\text{O}1$	178.4	177.5	$\text{C}7-\text{N}2-\text{C}8-\text{C}9$	-175.3	179.5
$\text{C}4-\text{O}1-\text{C}5-\text{O}2$	-3.4	-2.8	$\text{C}5-\text{N}1-\text{C}6-\text{C}7$	80.9	88.7
$\text{N}2-\text{C}7-\text{C}6-\text{N}1$	68.1	69.7	$\text{C}5-\text{O}1-\text{C}4-\text{C}3$	-59.3	-61.9

Table 4. Hydrogen-bond geometries (\AA , $^\circ$) for the titled compound

$\text{D}-\text{H}\cdots\text{A}$	$\text{D}-\text{H}$	$\text{H}\cdots\text{A}$	$\text{D}\cdots\text{A}$	$\text{D}-\text{H}\cdots\text{A}$
$\text{O}3-\text{H}3\cdots\text{N}2$	0.82	1.86	2.603 (6)	150
$\text{C}3-\text{H}3\text{C}\cdots\text{O}2$	0.96	2.35	2.969 (8)	122
$\text{C}2-\text{H}2\text{B}\cdots\text{O}2$	0.96	2.38	2.992 (8)	121
$\text{N}1-\text{H}1\cdots\text{O}2^i$	0.86	2.15	2.940 (5)	152

Symmetry codes: (i) $x, -y+1/2, z-1/2$.

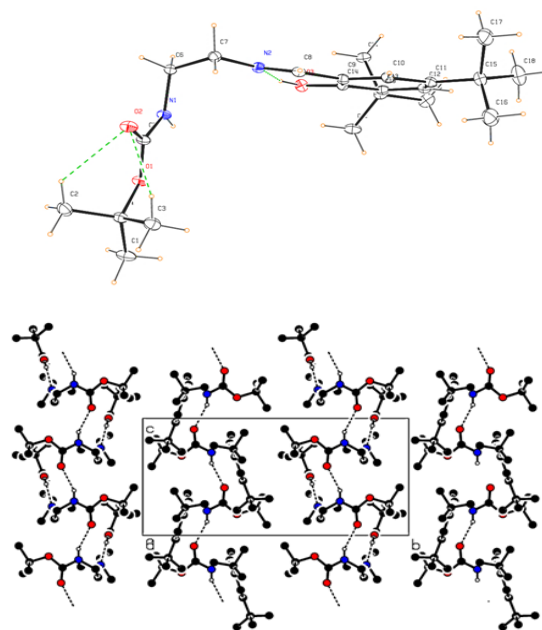


Fig. 5. (a) V-shaped conformation of the title compound, $\text{C}_{22}\text{H}_{36}\text{N}_2\text{O}_3$, indicates the intramolecular hydrogen bonds. H atoms are presented as small spheres of arbitrary radius. (b) In the crystal-packing diagram, the hydrogen bond is shown as dashed lines along with $\text{N}1-\text{H}1\cdots\text{O}2$ (green).

4. Conclusions

In this paper, (*E*)-*tert*-butyl (2-((3,5-*di-tert*-butyl-2-hydroxybenzylidene)amino)ethyl) carbamate has been synthesized and characterized by FT-IR, ¹H-NMR, ¹³C-NMR, MS, elemental analyses. The target compound (**3**) was obtained as single crystal suitable for X-ray analysis. All crystallographic data agree with the theoretical bond lengths, angles, dihedral angles of the target compound. The results of theoretical spectral analysis, ¹H-NMR, ¹³C-NMR and FT-IR are agreement with the experimental data.

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