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Synthesis, X-ray crystal structure and DFT study of potential ligands of (2*Z*)-3-[(2-hydroxyphenyl)amino]-1-phenyl"alk"-2-en-1-one type

Aneta Jezierska *, Lucjan B. Jerzykiewicz, Jerzy Kołodziejczak, Jarosław M. Sobczak

University of Wrocław, Faculty of Chemistry F. Joliot-Curie 14, 50-383 Wrocław, Poland

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Abstract

The main aim of the study was the synthesis and X-ray and spectroscopic investigations of potential ligands of transition metal complexes. A new compound, (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one, was obtained and the detailed experimental results are reported. Theoretical investigations based on the Density Functional Theory (DFT) were also performed for the presented compound as well as for its two analogues. Conformational analysis was done to find minima on the potential energy surface (PES). Analysis of the electrostatic potential (ESP) showed regions in the molecules sensitive to external interactions. Furthermore, topological analysis of the electron density (AIM theory) was applied to confirm the existence of an intramolecular H-bond in the molecules studied. The obtained theoretical results are in good agreement with the available experimental data.

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1. Introduction

Homogenous catalysis reactions are currently very important tools in the chemical industry and applied chemistry. The search for new potential ligands for catalytic complexes is important in developing faster and more efficient processes. In this paper, we would like to report experimental and theoretical results concerning the geometrical and electronic structure description of a new potential ligand of transition metal complexes, (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (marked as III). Additionally, the Molecular modeling section contains a discussion of two previously published compounds, N-(2-hydroxyphenyl)-4-amine-3-pentene-2-one and 3-[(3-hydroxyphenyl)amine]-1-phenylbut-3-en-1-one (marked as I and II, respectively), with similar structural parameters [1–3].

Generally, condensation reaction of β -diketones with primary amines (see Scheme 1) should lead to an iminoke-

tone form (Scheme 1, reaction 1), for which the occurrence of the iminoenol and aminoenone forms (Scheme 2, reaction 2) is assumed.

However, structural data (i.e. X-ray) show that, independently of the type of reacting substances, derivatives of aminoenones were obtained. For example, starting from 2,4-pentadione and o-aminophenol, N-(2-hydroxyphenyl)-4-amine-3-pentene-2-one (I) is prepared [1,4]. Benzoyloacetone is reacted with o-aminophenol to form 3-[(3-hydroxyphenyl)amine]-1-phenylbut-3-en-1-one (II), for which the three conformational forms (we will mark these as IIa, IIb, and IIc, respectively; see [3] for details) and the ethanol solvate (marked as IId) [2] have been found. Similarly, the reaction of benzovloacetone with 2-aminoethanol leads to 3-(hydroxyethyl)amine-1-phenylbut-2-en-1-one [5]. In the same way, o-aminophenol reacts with different benzoyl derivatives, e.g. 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone [6]. An analogous reaction proceeds in the case of 5,5-dimethylcyclohexane-1,3-dione with o-aminophenol [7]. This class of compounds, which exist as aminoenones, formed complexes with metals, in

^{*} Corresponding author. Tel.: +48 71 3757 308; fax: +48 71 3282 348. *E-mail address:* anetka@elrond.chem.uni.wroc.pl (A. Jezierska).

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Scheme 2. Scheme of the synthesis reaction pathway of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III).

which they can co-ordinate in monodentate or chelate structures. Examples are compounds of Co, Sn, the lanthanides [8], as well as Pd and U [9]. In the presence of an additional hydroxyl group (in the case of reactions of B-diketones with *o*-aminophenol or 2-aminoalcohols). potentially tridentate monobasic ligands can be formed. Such examples are titanium complexes with derivatives of N-(2-hydroxyethyl)-4-amine-3-pentene-2-one [10]. In order to support the experimental investigations and develop new models useful for further study, theoretical investigations were performed. In our case, calculations based on the Density Functional Theory (DFT) [11] were carried out to discuss the conformational flexibility of the molecules studied. The electronic structure description gives insight into the electrostatic potential distribution around the studied compounds showing atoms mostly involved into external interactions. Bader's analysis, in this case, was applied to investigate theoretically the presence of an intramolecular hydrogen bond [12–14].

2. Experimental and computational procedures

All the reagents and the solvents employed were commercially available and used with no further purification. Acetophenone (Aldrich), propionic acid (Koch-Light), and 2-aminophenol (Ferak) were used.

2.1. Preparation of 1-phenylpentane-1,3-dione

The title compound was obtained from acetophenone and ethyl propionate prepared according to the procedure described for benzoylacetone [15]. GC-MS analysis of the obtained crude oil shows three main peaks: unreacted acetophenone, 1-phenylpentane-1,3-dione (the highest peak), and 1,5-diphenylpentane-1,3,5-trione. The mixture was distilled under reduced pressure and pure title compound was collected (confirmed by GC-MS).

IR (film), cm⁻¹: ν (O–H) ca. 3000 m,br; ν (C–H) 3064 vw, 3031 vw, 2978 w, 2940 w, 2879 sh, 2740 vw; ν (O–H···O) ca. 2658 vw, br; ν (C=O), δ (O–H) and ν (C=C) 1720 m, 1686 m, 1604 vs, 1574 vs, 1492 m; δ (C–H) 1455 s, 1419 m, 1378 m; 1339 w; δ (C–O_{Ph}) 1270 s; 1180 m; 1155 m; 1085 w; 1068 m; 1043 w; 999 m; 930 w; 823 m; δ (C–C_{Ph}) 763 s, γ (C– H_{Ph}) 714 sh, 695 s; 668 w; 546 w.

¹H NMR (CDCl₃, at 20 °C): δ 0.95 (t, 3H, $-CH_3$), 2.2 (q, 4H, $-CH_2$ -Me), 5.92 (s, 1H, $=CH_-$), 7.2 (m, 3H, Ph), 7.6 (m, 2H, Ph).

2.2. Preparation of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III)

The title compound was obtained *via* condensation of 1phenylpentane-1,3-dione (3.2 mL, 0.02 mol) and 2-aminophenol (2.19 g, 0.02 mol) in absolute ethanol (20 mL). The mixture was refluxed for 3 h. Yellow-green crystals were formed during reflux. The crystals were collected, washed with alcohol, and dried in vacuum to yield 3.22 g (60.2%) of the title compound (m.p. = 188.5-189.5 °C).

Anal. Calcd for C₁₇H₁₇NO₂: C, 76.38; H, 6.41; N, 5.24. Found: C, 76.1; H, 6.7; N, 5.3.

IR (KBr disk), cm⁻¹: v(O–H) 3435 w,br; v(C–H) 3089 m,br, 2974 m, 2934 w, 2873 w, 2730 w, 2595 vw; v(C=O), δ (N–H) and v(C=C) 1602 s, 1576 vs, 1540 m, 1516 s; δ (C–H) 1458 s, 1378 m, 1334 s, 1281 s; 1249 m; δ (C–O_{Ph}) 1226 s; v(C–N) 1178 s; 1102 m; 1071 m; 1052 m; 942 w; 857 w; 827w, 806 w; δ (C–C_{Ph}) 755 s; γ (C–H_{Ph}) 702 m; 688 w; 648 m; 539 w; 503 w; 464 w; 444 w; 417 vw; 402 w.

UV–vis (MeOH) $[\lambda_{max}/nm (\epsilon/M^{-1} cm^{-1})]$: 352 (15100), 246 (9300), 208 (16900).

¹H NMR (CDCl₃, at 20 °C): δ 0.8 (t, 3H, -*CH*₃), 2.0 (q, 4H, -*CH*₂-), 5.72 (s, 1H, =*CH*-), 6.8 (m, 1H, *H*_{Ph}), 7.0 (m, 2H, *H*_{Ph}), 7.1 (m, 1H, *H*_{Ph}), 7.4 (m, 4H, *H*_{Ph} and -*NH*-), 7.8 (m, 2H, *H*_{Ph}), 12.3 (s, 1H, -*OH*).

¹³C NMR (CDCl₃, at 20 °C): δ 10.2 (-CH₃); 24.1 (-CH₂-); 90.9 (= CH-); 115.3, 118.7, 123.2, 125.4, 125.7, 126.7, 127.1, 127.4, 129.5, 130.7, 138.5, 150.8 (C_{Ph}); 168.9 (\equiv C-NH-); 187.7 (=C=O).

2.3. Physical measurements

IR spectra were measured using an Impact 400 (Nicolet) FT-IR spectrophotometer. UV-vis electronic spectra were obtained using Hewlett Packard Model 8452A Diode Array spectrophotometers. ¹H and ¹³C NMR spectra were recorded on a Bruker 300 spectrometer. A Hewlett Packard 5890 II series gas chromatograph coupled with a Hewlett Packard Model 5971A mass selective detector was used for the GC/MS analyses. Elemental analyses were performed in the Microanalytical Laboratory of the Faculty of Chemistry, University of Wrocław. Melting points were obtained on a Boëtius apparatus and are uncorrected.

2.4. Determination and refinement of the structure

Preliminary examination and intensity data were determined on a Kuma KM4CCD κ -axis diffractometer with graphite-monochromated MoK α radiation ($\lambda =$ 0.71073 Å). For all data, Lorentz and polarization corrections were applied. The structures were solved by direct methods and refined by the full-matrix least-squares method on all F^2 data using the SHELXTL 5.0 package [16]. Carbon-bonded hydrogen atoms were included in the calculated positions and refined in the riding mode using SHELXTL default parameters. Other hydrogen atoms were located in a difference map and refined freely. Full crystallographic details of the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 290376. Copies of the data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk). Additionally, the crystallographic data are also available on request from the Authors.

2.5. Computational methodology

The Density Functional Theory (DFT) proposed by Hohenberg and Kohn was applied in order to investigate the geometrical parameters and the electronic structure of the molecules studied [11,17]. Nonlocal three-parameter hybrid exchange and correlation functional proposed by Becke in conjugation with the Lee-Young-Parr correlation formula (B3LYP) was used during the theoretical investigations [18,19]. The 6-31G(d,p) double-zeta basis set with polarization functions on both heavy and hydrogen atoms [20] was applied during the conformational analysis. For each of the molecules studied, a one-dimensional potential energy surface (PES) scan was performed by variation of selected dihedral angles (24 steps with 15° increments and full geometry optimization during the conformational search). The conformers corresponding to the minimum on the PES were obtained and the basis set was furthermore enlarged to 6-311+G(d,p) [21–23]. The obtained structures were re-optimized and the vibrational frequencies were calculated, confirming that the geometrical parameters correspond with a minimum, not a saddle point. In the next step, the electrostatic potential (ESP) and Kohn-Sham determinant pseudo-wavefunction for Atoms in Molecules (AIM) [12-24] were calculated using the triple-zeta 6-311+G(d,p) basis set. Molecular modeling in silico was performed using the Gaussian03 series of programs [25]. Topological analysis of the electron density according to Bader theory was performed using the AIM-PAC package [26]. Visualization of the obtained results was achieved with the help of the Molekel [27] and gOpen-Mol [28] programs.

3. Results and discussion

3.1. Synthesis and X-ray crystal structure discussion

The Claisen condensation reaction between acetophenone and ethyl propionate followed by distillation under low pressure gave 1-phenylpentane-1,3-dione. Treatment of this compound with one equivalent of o-aminophenol in refluxing ethanol for 3 h produced (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III) (Scheme 2).

Both of the prepared compounds were studied using NMR, IR, and UV–vis spectroscopic methods. In the ¹H NMR spectrum of a CDCl₃ solution of 1-phenylpentane-1,3-dione, the signal of the methine proton at 5.92 ppm points at a predominance of the enol form. Similarly, the ¹H NMR spectrum of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III) shows the signals of the

methine proton at 5.72 ppm and of the N–H proton at ca. 7.4 ppm, pointing at the existence of the aminoenone form. For these compounds, inter- and intramolecular hydrogen bonds were observed in solid state and in IR spectrum (broad absorption in the range of $3300-2600 \text{ cm}^{-1}$).

Besides the spectroscopic investigations, the crystal structure was also determined using X-ray crystallography. A single crystal of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (**III**) suitable for X-ray structure analysis was obtained (Fig. 1).

Crystal data and structure refinement details for (III) are presented in Table 1.

The X-ray structure showed that the dihedral angles between the N8–C9=C12–C13=O14 plane and the benzene and substituted benzene rings are 28.40(8)° and 67.35(9)°, respectively. For a similar compound, i.e. 3-[(3hydroxyphenyl)amine]-1-phenylbut-3-en-1-one (II), for which the three conformational forms and the ethanol solvate were found (IIa–d), the same dihedral angles are $17.99(7)^{\circ}$ and $41.52(8)^{\circ}$ for IIa, $14.36(9)^{\circ}$ and $57.05(8)^{\circ}$ for IIb, $27.60(9)^{\circ}$ and $84.64(3)^{\circ}$ for IIc [3], and $21.96(13)^{\circ}$ and $46.68(13)^{\circ}$ for IId (ethanol adduct) [2]. This is a proof of the flexibility of the investigated molecular skeleton, which will also be evident in the calculated rotational profiles. Because of the steric repulsion between the monosubstituted phenyl ring and ethyl group, the rotation of the ring is hindered. The distance between the O7 atom and C11 of the ethyl group is 3.945(3) Å. The proton donor group N8–H21 forms an intramolecular hydrogen bond with oxygen atom O14, with a bond length of 2.633(2) Å and a valence angle of $144(2)^{\circ}$ (Table 2).

An intermolecular H-bond, O7–H22 \cdots O14, of length 2.653(3) Å and valence angle $172(2)^{\circ}$ is also observed. Because of this hydrogen bond, zig-zag chains are formed. The presence of the H-bond appears as an important property of the molecule, stabilizing its conformation in the crystal; as shown in the Molecular modeling part, this is also visible in the model obtained for the molecule discussed.

3.2. Computational study

The structures of the compounds discussed, with the atom numbering scheme used during the computational investigations, are presented in Fig. 2.

The conformational analysis of the studied molecules was performed based on the DFT and at the B3LYP/6-31G(d,p) level. During the conformational study, special attention was focused on the phenyl and phenolic ring rotations in all of the studied compounds (I, II, and III). For compound III the rotation of the ethyl group was also taken into account as an important feature for discussing the steric effects in the molecule. Additionally, the values obtained for the electron density and its Laplacian at the



Fig. 1. The molecular structure of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one with atom numbering scheme (III).

37

Table 1 Crystal data and structure refinement details for (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III)

Compound	(2Z)-3-[(2-Hydroxyphenyl)amino]-1-		
-	phenylpent-2-en-1-one		
Formula	$C_{17}H_{17}NO_2$		
Μ	267.32		
$T(\mathbf{K})$	100(2)		
Crystal system	Monoclinic		
Space group	P 2 ₁		
a (Å)	8.524(3)		
b (Å)	9.866(3)		
<i>c</i> (Å)	8.796(3)		
β (°)	102.89(3)		
$U(\text{\AA}^3)$	721.1(4)		
Ζ	2		
$D_c(\mathrm{g\ cm^{-3}})$	1.231		
$\mu (\mathrm{mm}^{-1})$	0.081		
$\theta_{\min} - \theta_{\max}$ (°)	3.01 to 27.49		
Reflections measured	5751		
Unique reflections	1729		
R _{int}	0.0276		
Observed reflections $[I \ge 2\sigma(I)]$	$1501[I > 2\sigma(I)]$		
Parameters	189		
R_1 (observed reflections)	0.0332		
wR_2 (all reflections)	0.0732		
S	1.066		
$\Delta \rho_{\rm max}; \ \Delta \rho_{\rm min} \ ({\rm e. \AA}^{-3})$	0.188; -0.146		

bond critical point (BCP) between proton and acceptor based on AIM theory supported our study, proving theoretically the presence of an intramolecular hydrogen bond according to the criteria of Koch and Popelier [14]. The electrostatic potential surface (ESP) analysis gave insight into the electronic structure of these three compounds, showing places potentially involved in complex formation.

The variation of the dihedral angle (C2-C1-N8-C9) and the OH group position of *N*-(2-hydroxyphenyl)-4-amino-3-penten-2-one (I) was analyzed and the obtained results are presented in Fig. 3.

Two symmetry-related minima were found for 60° and 150° with a small barrier between them (1 kcal/mol). A much higher barrier (6 kcal/mol) is present when the OH group of the phenolic ring passes closely to the methyl group. Both conformers are almost identical with respect to energy, although lower energy was obtained for the 60° structure (the –OH group of the phenolic ring is in *syn* position with respect to the methyl group). The small



Fig. 2. The structures of the theoretically investigated compounds with atom numbering scheme. (A) *N*-(2-Hydroxyphenyl)-4-amino-3-penten-2-one (I). (B) 1-Phenyl-3-(2-hydroxyphenylamino)-2-buten-1-one (II). (C) (2*Z*)-3-[(2-Hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III).

rotational barrier enables an easy exchange between these two conformers. This is important because of their different coordination abilities (discussed below).

The theoretical results confirming the presence of the intramolecular hydrogen bond are presented in Table 3. The obtained electron density and its Laplacian at the hydrogen bond critical point (BCP) have quite large values

Table 2

Experimental and theoretical hydrogen bond parameters for (2Z)-3-[(2-hydroxy-phenyl)amino]-1-phenylpent-2-en-1-one (III) (Å and °)

D–H···A	d(D-H)	$d(\mathbf{H} \cdot \cdot \cdot \mathbf{A})$	$d(\mathbf{D} \cdot \cdot \cdot \mathbf{A})$	<(DHA)
Experimental intra- and intermo	lecular hydrogen bond parame	ters		
$N(8) - H(21) \cdots O(14)$	0.90(2)	1.86(2)	2.633(2)	144(2)
O(7)−H(22)···O(14)#1	0.92(3)	1.74(3)	2.653(2)	172(2)
Theoretical intramolecular hydro	ogen bond parameters (DFT, E	B3LYP/6-31G(d,p), and $B3LY$	P/6-311+G(d,p), respectively)	
$N(8)-H(21)\cdots O(14)$	1.0327	1.7418	2.6181	139.97
	1.0296	1.7712	2.6307	138.31

Symmetry transformations used to generate equivalent atoms: #1 - x, y + 1/2, 1 - z.



Fig. 3. Results of the one-dimensional relaxed B3LYP/6-31G(d,p) conformational search of the studied compounds. The conformational search consisted of 24 steps (geometry optimization) with 15° increases in the indicated dihedral angle at each step. *N*-(2-Hydroxyphenyl)-4-amino-3-penten-2-one (I). The variation of the C2–C1–N8–C9 dihedral angle (top). 1-Phenyl-3-(2-hydroxyphenylamino)-2-buten-1-one (II). The variation of the dihedral angle C2–C1–N8–C9 (middle left) and C15–C14–C12–O13 (middle right). (2*Z*)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III). The variation of the dihedral angle H22–O7–C2–C3 (bottom left) and C11–C10–C9–C12 (bottom right).

typical for compounds with this kind of rather short hydrogen bond according to the criteria proposed by Koch and Popelier [14].

Table 3

Electron density and its Laplacian at the bond critical point (BCP) between proton and acceptor of the intramolecular hydrogen bond based on B3LYP/6-311+G(d,p)

BCP parameters	(I)	(II)	(III)
$\rho [e/a_0^3]$	0.04044	0.04116	0.04202
$\nabla^2 \rho \ [e/a_0^5]$	+0.13204	+0.13507	+0.13683

Electrostatic potential (ESP) maps (see Fig. 4) were obtained for both conformers in order to show the difference in their complexation ability.

The structure, with the OH and methyl groups in *anti* position, is clearly a bi- or tridentate ligand because of the large region of negative ESP caused by favorable arrangement of the O7, N8, and O13 atoms. Because of the rotational freedom and small energy difference between these two conformers, the mode of coordination described above should be generally preferred in the metal complexes of (I). The presence of the hydrogen bond in the ligand



Fig. 4. The electrostatic potential (ESP) for the analyzed compounds (I, II, and III, respectively). Dark gray marks regions of decrease -0.05 a.u. and light gray of increase 0.6 a.u. (A) The electrostatic potential (ESP) for a conformer with a minimum at 60° (above) and at 150° (below) for *N*-(2-Hydroxyphenyl)-4-amino-3-penten-2-one (I). (B) 1-Phenyl-3-(2-hydroxyphenylamino)-2-buten-1-one (II). (C) (2Z)-3-[(2-Hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III).

structure additionally stabilizes both conformations; moreover, it facilitates proton removal from the nitrogen atom, which finally leads to tridentate dibasic ligands.

The conformational analysis of 1-phenyl-3-(2-hydroxy-phenylamino)-2-buten-1-one (II) was also performed as a first step of the theoretical study of the compound. The

variations in the phenol, phenolic ring, and OH group positions were taken into account during the study. The obtained results are presented in Fig. 3. The most stable conformer has the same atomic arrangement as the X-ray structure reported in the literature [3]. The phenolic ring rotation energy profile shows three minima (at ca. -160° , -90° , and $+120^{\circ}$, respectively), but one of the rotation barriers is 10 kcal/mol, which suggests a strong steric repulsion between the OH and methyl groups. The phenyl ring has two preferred conformations, which are in fact symmetrical and equivalent $(-30^{\circ} \text{ and } +150^{\circ})$. The presence of the hydrogen bond (between atoms N8-H20...O13) was confirmed theoretically as shown in Table 3. The ESP distribution (see Fig. 4) indicates that (II) is also likely to act as a tridentate ligand. The concentration of the negative ESP is visible between atoms containing lone electron pairs. The carbonyl group and OH group from the phenolic ring have a significant contribution and the negative ESP is localized between these two groups.

The conformational flexibility of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III) was studied by analysis of the phenol and phenolic rings and OH and ethyl group positions. The most stable conformer has an atomic arrangement similar to the structure obtained by X-ray diffraction (compare Figs. 1 and 2; the geometry shown in Fig. 2 was obtained at the B3LYP/6-311+G(d,p) level). The structural parameters obtained from the computational study are in good agreement with the experimental data. The only significant difference is the relative arrangement of the ethyl group and the phenolic ring, which was found to be very flexible in the conformational analysis. In Fig. 3 are presented one-dimensional energy profiles obtained by variation of the dihedral angles containing the OH group from the phenolic ring and the ethyl group, respectively, in the molecule studied. The conformer with the lowest energy was taken as a structure in the minimum on the PES and investigated further. The observed discrepancies between experimental and theoretical results, especially in some flexible torsion angles, are caused by gas-phase modeling which neglects the environmental (steric, electrostatic, and H-bond) influence of the neighboring molecules. It is significant to note that the obtained models are in good agreement with the available experimental data. The presence of an intramolecular hydrogen bond was confirmed experimentally and theoretically (see Tables 2 and 3, respectively). The obtained theoretically distances between the atoms involved in the hydrogen bond and the value of the valence angle are in quite good agreement with the experimental data. The analysis of electron density and its Laplacian at the hydrogen bond critical point have quite large values, which proves the presence of the bond analyzed based on criteria proposed for such a type of bonding [14]. The electrostatic potential shows that the atoms with lone electron pairs are in neighboring positions with respect to each other (see Fig. 4), so the negative ESP is cumulated and the compound could also act as a potentially tridentate ligand.

The theoretical electronic structure analysis showed that the molecules studied have very similar properties and should form complexes with similar catalytic properties. The results obtained theoretically describing the geometrical and electronic structure parameters are useful for further experimental study. They highlight the bonding possibilities during complex formation.

4. Conclusions

We have been successful in synthesizing the potential of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenyl" ligands alk"-2-en-1-one type. The details of synthesis, spectroscopic data, and crystal structure of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one (III) are presented. Additionally, quantum-chemical investigations based on the DFT method were performed for the molecule discussed (III) and its two analogues (I and II) in order to study the physico-chemical nature of these compounds, especially conformational flexibility and the electrostatic potential surface. The experimentally obtained results are in good agreement with theory and the models proposed are useful for our future studies. The work is still in progress and as a next step we would like to investigate the synthesis and structure of metal complexes and their catalytic activity.

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