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# Correlation between single crystal data and molecular mechanics calculation of 3-(2-hydroxy-phenylimino)-1,3-diphenyl-propan-1-one

 Adel Sayed Orabi <sup>1</sup> and Sahar Said El-Sakka <sup>2,\*</sup>
<sup>1</sup> Chemistry Department, Faculty of Science, Suez Canal University, Ismailia 41522, Egypt  
[orabiadel@hotmail.com](mailto:orabiadel@hotmail.com) (A.S.O.)

<sup>2</sup> Chemistry Department, Faculty of Science, Suez University, Suez 43527, Egypt  
[sahar.alsakka@suezuniv.edu.eg](mailto:sahar.alsakka@suezuniv.edu.eg) (S.S.E.)

 \* Corresponding author at: Chemistry Department, Faculty of Science, Suez University, Suez 43527, Egypt.  
 Tel: +20.100.6054033 Fax: +20.62.3707040 e-mail: [sahar.alsakka@suezuniv.edu.eg](mailto:sahar.alsakka@suezuniv.edu.eg) (S.S. El-Sakka).

## RESEARCH ARTICLE

## ABSTRACT



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The Schiff base 3-(2-hydroxy-phenylimino)-1,3-diphenyl-propan-1-one (L), was prepared and characterized by elemental analysis, IR, <sup>1</sup>H NMR and mass spectral techniques. The crystal and molecular structures were determined by using the single crystal X-ray diffraction data. The crystal was triclinic with unit-cell dimensions:  $a = 9.051(3) \text{ \AA}$ ,  $b = 10.245(3) \text{ \AA}$ ,  $c = 11.016(3) \text{ \AA}$ ,  $\alpha = 69.28(2)^\circ$ ,  $\beta = 81.66(2)^\circ$ ,  $\gamma = 64.25(2)^\circ$ , space group is  $P\bar{1}$  and  $Z = 2$ . The structure was refined by least squares method. The single crystal was prepared by supersaturating method using tetramethoxysilane as gelling agent. Energy minimization for locating stable conformations and single point energy calculations for comparing the obtained and calculated conformations of the same molecule were carried out using molecular mechanics method (MM2 force field). The bond lengths and the bond angles were calculated and compared with the values obtained from the single crystal analysis. The obtained results were discussed and evaluated. Generally, the calculated parameters are in good agreement with the corresponding X-ray diffraction values. The obtained results reveal that, the amine-imine tautomerism is more preferable than keto-enol form and the intra-hydrogen bond stabilize the amine-imine tautomerism.

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## 1. Introduction

The preparation and characterization of the single crystal of the organic compounds, especially, Schiff bases have gained much attention, likely due to the versatile applications of the well characterized Schiff bases [1-4]. The single crystal of the Schiff base (L) was prepared by using sol-gel method using tetramethoxysilan (TMOS) as gelling agent. In such system, several self-regulation mechanisms enhance the crystal growth of low solubility and low thermal stability materials. TMOS was slightly more favorable than the other gelling agents, may be, due to: (a) compatible with the pH range of the experiment, (b) compatible with the oxidizing or reducing properties of the reagents used and (c) has ability to give minimum unwanted side reactions [5-7].

The theoretical calculation of the molecular structure by using different computational methods allows the exploration of molecules through the use of a computer in cases when an actual laboratory investigation may be inappropriate, impractical, or impossible. As an adjunct to experimental chemistry, its significance continues to be enhanced by explosive increases in computer speed and power. The molecular mechanics MM2 force fields method with minimum

RMS gradient = 0.1 (using CS Chem3D 7.0 which stand alone as application within the package program CS-ChemOffice was used to improve: (a) The Energy minimization for locating stable conformations, (b) Single point energy calculations for comparing conformations of the same molecule and (c) Searching conformational space by varying a single dihedral angle [8-15].

## 2. Experimental

### 2.1. Reagents

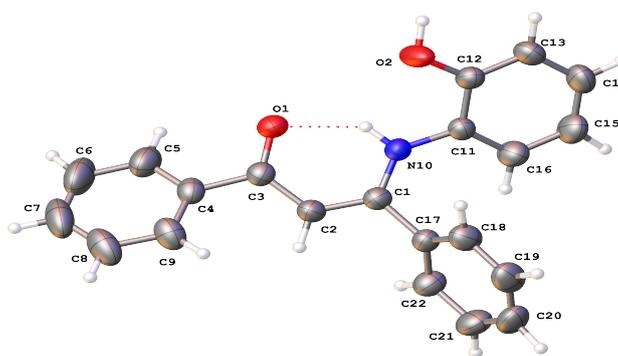
All chemicals used were of reagent grade; organic solvents were purified by standard methods.

### 2.2. Instrumentation

Infrared spectra were recorded in the range of 4000 to 200  $\text{cm}^{-1}$  using KBr disc technique on a Perkin-Elmer 883 spectrophotometer. <sup>1</sup>H-NMR spectra of the synthesized compound was obtained using Bruker AC 200 spectrometer, 200 MHz with tetramethylsilane (TMS) as internal standard.

**Table 1.** Single crystal X-ray crystallographic analysis of the synthesized compound (L).

Identification code	883173
Empirical formula	C <sub>21</sub> H <sub>17</sub> NO <sub>2</sub>
Formula weight	315.36
Temperature (K)	293
Crystal system	Triclinic
Space group	P-1
a (Å)	9.051(3)
b (Å)	10.245(3)
c (Å)	11.016(3)
α (°)	69.28(2)
β (°)	81.66(2)
γ (°)	64.25(2)
Volume (Å <sup>3</sup> )	860.5(4)
Z	2
ρ <sub>calc</sub> (g/cm <sup>3</sup> )	1.217
μ (mm <sup>-1</sup> )	0.078
F(000)	332.0
Crystal size (mm <sup>3</sup> )	1.000 × 0.375 × 0.375
Radiation	MoKα (λ = 0.71069)
2θ range for data collection (°)	4.66 to 55.98
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	4143
Independent reflections	4364 [R <sub>int</sub> = 0.0175]
Data/restraints/parameters	4364/0/285
Goodness-of-fit on F <sup>2</sup>	1.057
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0425, wR <sub>2</sub> = 0.1304
Final R indexes [all data]	R <sub>1</sub> = 0.0676, wR <sub>2</sub> = 0.1394
Largest diff. peak/hole (e Å <sup>-3</sup> )	0.20 and -0.23

**Figure 1.** ORTEP diagram of the single crystal of the synthesized ligand.

Elemental analysis was carried out using a Heraeus CHN-Rapid Analyzer. Mass spectra of the synthesized Schiff base were obtained with a mass spectrometer Varian Mat 711. Single crystal X-ray analysis was carried out on STOE diffractometer using a MoKα source (λ = 0.71069 Å). Photographs of the crystals were obtained using a SZ-PT Olympus microscope fitted with an Olympus camera (Univ. Ulm, Germany). The structure was solved by direct methods and refined by least square cycles. All calculations and drawing were performed using the SHELX and ORTEP programs [16]. The crystallographic data for the titled compound are listed in Table 1.

### 2.3. Preparation of the single crystal

#### 2.3.1. Preparation of crude compound

The Schiff base 3-(2-hydroxy-phenylimino)-1,3-diphenylpropan-1-one (L), was prepared (powder) as described previously [17]. Color: Orange. Yield: 80%. M.p.: 197-199 °C. FT-IR (ν, cm<sup>-1</sup>): 3370 (s), 3310 (s) (OH); 2710, intramolecular hydrogen bond; 1600, 1560 (m) (C=O, C=N). <sup>1</sup>H NMR (200 MHz, DMSO-*d*<sub>6</sub>, δ, ppm): 12.67 (s, 1H, OH), 10.10 (s, 1H, enol-OH), 8.00-6.22 (m, 14H, aromatic), 6.20 (s, 1H, =CH-). MS (*m/z* (%)): 315 (20) (L<sup>+</sup>). Anal. calcd. for C<sub>21</sub>H<sub>17</sub>NO<sub>2</sub>: C, 79.98; H, 5.43; N, 4.44. Found: C, 79.95; H, 5.55; N, 4.87%.

#### 2.3.2. Preparation the gel solution

The solution of the gel was prepared by mixing 10 mL TMOS with 90 mL water. The mixing proceeds by adding TMOS to water with stirring. Fill the clean tubes (20 cm length with minimum diameter equal 2 cm) by the prepared gel sol nearly to half its length and leave it for 24 hr to allow the gelling proceed [18].

#### 2.3.3. Preparation the gel-Schiff base mixture

Saturated solution from the Schiff base was prepared by dissolving the titled compound using ethanol-water mixture (with minimum ethanol %) then, mix it with freshly prepared gel solution. The formed mixture was used to refilling the second half of tube which previously prepared. Cover the tube by Parafilm paper (M) and let at stable bench.

### 3. Result and discussion

The single crystal of the synthesized compound (L) was grown by supersaturation method using TMOS as gelling agent at ambient temperature. Table 1 gives the crystal data and structure refinement. The ORTEP drawing is illustrated in Figure 1. Also, the package at different planes was shown in Figures 2-4 for the plane (011), (101) and (110), respectively. The package at (111) plane is illustrated in Figure 5.

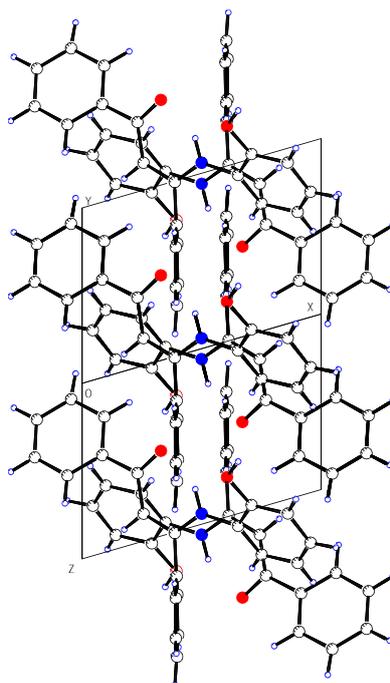


Figure 2. ORTEP diagram of the plane (011).

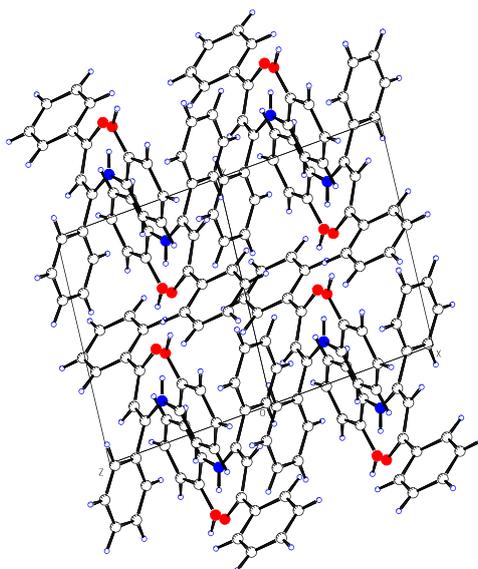


Figure 3. ORTEP diagram of the plane (101).

The atomic coordinates and equivalent isotropic thermal parameters were listed in Table 2. The bond lengths and angles are listed in Table 3 and 4, respectively. The photographic picture of the synthesized compound was represented in Figure 6. The listed atomic number label followed the number produced from the single crystal analysis data. Figure 7 shows the conformation of (L) compound after acting the energy minimization process. The sources of the steric energy which produced by MM2 force field method on the (L) compound and the related structures which produced from the tautomerism were listed in Table 5.

The calculated bond length  $g_0$  well with the experimental results with average deviation equal 0.02 Å with some exception, which the deviation reached to 0.17 Å. The variation ( $\Delta$ ) between the measured and calculated value ( $\Delta = \text{Experimental value (found)} - \text{Calculated value}$ ), generally has

negative value, which indicated that, the calculated bond length is slightly larger than the experimental one. The negative difference could be discussed in term of packing of the molecules in the crystal structure generate some  $\pi$ - $\pi$  interaction due to the stacking effect of the phenyl rings in the side chine of the molecules. The bonds which gave the largest  $\Delta$  were the carbon-hydrogen bonds of the phenyl rings and the N(10)-H(10) bond.

The bond angles, of the skeleton carbon, nitrogen and oxygen atoms, which obtained from the single crystal analysis nearly coincidence with the calculated value. Meanwhile the bond angles which contain hydrogen atom gave some variation nearly equal 6°. The variation could be due to the intra and inter-stacking effect which induce the non-1.4VDW, 1.4VDW and dipole-dipole interactions, which are larger in the package molecules.

**Table 2.** Atomic coordinates and equivalent isotropic thermal parameters.

Atom	x	y	z	U <sub>eq</sub>
O(1)	0.3290(1)	0.3968(1)	0.9112(1)	51(1)
C(16)	0.7509(1)	-0.0439(1)	1.2283(1)	53(1)
C(11)	0.6519(1)	0.1119(1)	1.1818(1)	40(1)
N(10)	0.4996(1)	0.1771(1)	1.1171(1)	45(1)
C(13)	0.8598(1)	0.1639(2)	1.2450(1)	53(1)
C(1)	0.3869(1)	0.1221(1)	1.1274(1)	41(1)
C(4)	0.0838(1)	0.4073(1)	0.8493(1)	46(1)
C(12)	0.7084(1)	0.2163(1)	1.1893(1)	45(1)
C(3)	0.2307(1)	0.3337(1)	0.9357(1)	43(1)
O(2)	0.6054(1)	0.3662(1)	1.1401(1)	74(1)
C(2)	0.2563(1)	0.1963(1)	1.0404(1)	45(1)
C(17)	0.3949(1)	-0.0164(1)	1.2385(1)	42(1)
C(15)	0.9015(2)	-0.0950(2)	1.2844(1)	62(1)
C(18)	0.3914(2)	-0.0146(1)	1.3644(1)	54(1)
C(20)	0.3964(2)	-0.2660(2)	1.4476(1)	71(1)
C(22)	0.3973(2)	-0.1429(2)	1.2179(1)	52(1)
C(8)	-0.1991(2)	0.4706(2)	0.8133(2)	80(1)
C(19)	0.3914(2)	-0.1397(2)	1.4684(1)	67(1)
C(14)	0.9554(1)	0.0083(2)	1.2934(1)	60(1)
C(21)	0.4004(2)	-0.2687(2)	1.3234(2)	66(1)
C(9)	-0.0624(2)	0.3941(2)	0.8941(1)	61(1)
C(7)	-0.1903(3)	0.5571(2)	0.6885(2)	90(1)
C(5)	0.0919(2)	0.4957(2)	0.7219(1)	68(1)
C(6)	-0.0468(3)	0.5698(2)	0.6419(2)	92(1)
H(16)	0.7112(18)	-0.1151(17)	1.2174(14)	65(4)
H(22)	0.3972(20)	-0.1425(18)	1.1290(16)	73(4)
H(18)	0.3867(18)	0.0823(18)	1.3769(14)	68(4)
H(2)	0.1756(15)	0.1525(14)	1.0547(12)	49(3)
H(21)	0.4018(19)	-0.3563(19)	1.3060(15)	75(4)
H(9)	-0.0727(20)	0.3366(19)	0.9915(16)	79(5)
H(13)	0.8939(18)	0.2407(18)	1.2536(15)	71(4)
H(19)	0.3932(22)	-0.1372(20)	1.5576(19)	88(5)
H(15)	0.9663(21)	-0.2079(21)	1.3077(16)	82(5)
H(2')	0.6523(21)	0.4325(20)	1.1357(16)	81(5)
H(14)	1.0618(19)	-0.0265(16)	1.3293(14)	62(4)
H(8)	-0.2995(40)	0.4590(31)	0.8445(28)	150(9)
H(5)	0.1963(19)	0.5028(18)	0.6886(15)	68(4)
H(20)	0.3881(28)	-0.3500(26)	1.5213(24)	124(7)
H(6)	-0.0279(25)	0.6223(25)	0.5556(22)	107(6)
H(7)	-0.2870(29)	0.6099(27)	0.6359(23)	121(7)
H(10)	0.4728(18)	0.2696(18)	1.0594(15)	64(4)

**Table 3.** The obtained and calculated bond length (Å) data.

Bond	Found	Calculated	Δ	Bond	Found	Calculated	Δ
O(1)-C(3)	1.2603(13)	1.233	0.027	C(15)-C(14)	1.380(2)	1.394	-0.014
C(16)-C(15)	1.382(2)	1.395	-0.013	C(15)-H(15)	1.00(2)	1.103	-0.103
C(16)-C(11)	1.388(2)	1.404	-0.016	C(18)-C(19)	1.384(2)	1.395	-0.011
C(16)-H(16)	0.988(14)	1.098	-0.110	C(18)-H(18)	1.03(2)	1.103	-0.073
C(11)-C(12)	1.400(2)	1.408	-0.008	C(20)-C(21)	1.372(2)	1.395	-0.023
C(11)-N(10)	1.4148(14)	1.413	0.002	C(20)-C(19)	1.374(2)	1.397	-0.023
N(10)-C(1)	1.3395(13)	1.390	-0.051	C(20)-H(20)	0.97(2)	1.102	-0.132
N(10)-H(10)	0.88(2)	1.052	-0.172	C(22)-C(21)	1.390(2)	1.400	-0.010
C(13)-C(14)	1.381(2)	1.397	-0.016	C(22)-H(22)	0.98(2)	1.102	-0.122
C(13)-C(12)	1.384(2)	1.398	-0.014	C(8)-C(7)	1.359(3)	1.397	-0.038
C(13)-H(13)	1.00(2)	1.102	-0.102	C(8)-C(9)	1.387(2)	1.395	-0.008
C(1)-C(2)	1.387(2)	1.368	0.019	C(8)-H(8)	0.97(3)	1.103	-0.133
C(1)-C(17)	1.4916(14)	1.492	0.000	C(19)-H(19)	0.99(2)	1.103	-0.113
C(4)-C(5)	1.387(2)	1.403	-0.016	C(14)-H(14)	0.96(2)	1.102	-0.142
C(4)-C(9)	1.390(2)	1.404	-0.014	C(21)-H(21)	0.98(2)	1.102	-0.122
C(4)-C(3)	1.494(2)	1.494	0.000	C(9)-H(9)	1.04(2)	1.101	-0.061
C(12)-O(2)	1.3542(14)	1.362	-0.008	C(7)-C(6)	1.369(3)	1.395	-0.026
C(3)-C(2)	1.418(2)	1.478	-0.060	C(7)-H(7)	0.95(2)	1.102	-0.152
O(2)-H(211)	0.93(2)	0.971	-0.041	C(5)-C(6)	1.395(2)	1.397	-0.002
C(2)-H(2)	0.980(12)	1.102	-0.122	C(5)-H(5)	0.99(2)	1.102	-0.112
C(17)-C(22)	1.383(2)	1.398	-0.015	C(6)-H(6)	0.95(2)	1.102	-0.152
C(17)-C(18)	1.390(2)	1.401	-0.011				

Δ = Experimental value (found) - calculated value.

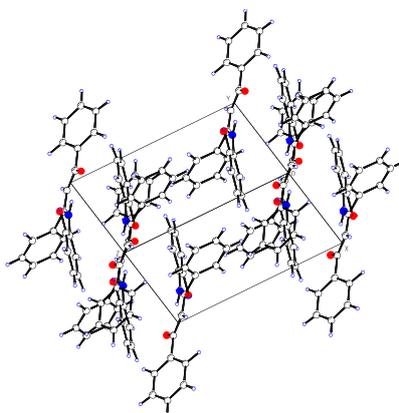
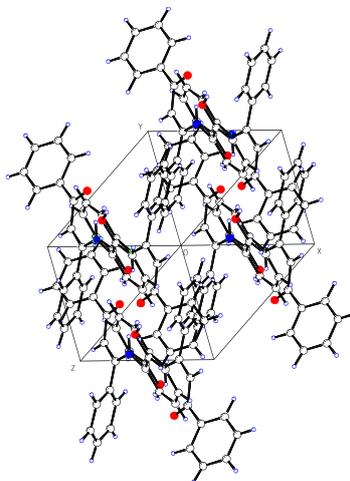
Figures 2-5 are illustrated the array of the molecules with different view for different planes with indices as (011), (101) and (110) for two directional view and as (111) for packing molecules for three directional view. All these Figures gave some idea about the strength of the stacking which present among the molecules in the crystal lattice.

The calculated Steric energy (kcal/ mol) for the synthesized Schiff base and its tautomer using MM2 force field method was carried out to clarify and introduce some evidence about the nature of the most stable tautomer. Table 5

and Figure 7 are illustrated the L-compound, L-keto-enol and L-amine-imine tautomerisms. From Table 5, could be deduce the order of the steric energy type as: 1.4VDW ≥ Torsion > Non-1.4VDW ≥ Bend > Dipole-dipole ≥ Stretch > Stretch-bend. So, the most effective parameters are 1.4VDW, Torsion, Non-1.4VDW and Bend. Meanwhile, the least effective parameter is Stretch-bend. The 1.4VDW values are 11.432, 12.956 and 10.651 kcal/ mol for L-keto-enol, L-compound and L-amine-imine, respectively.

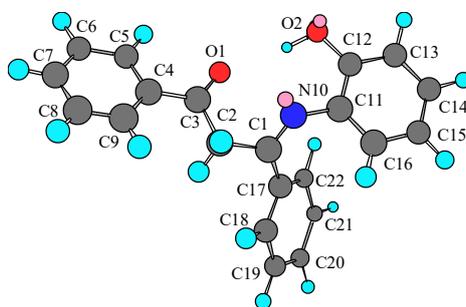
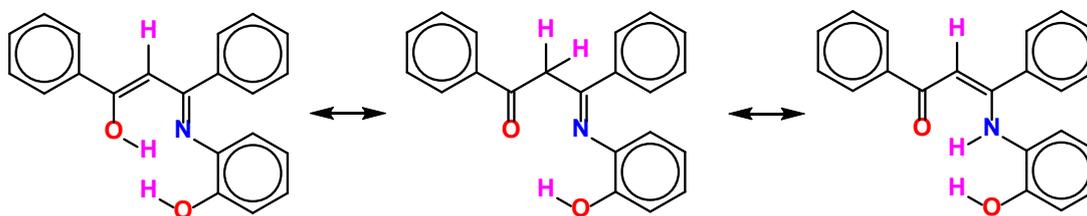
**Table 4.** The obtained and calculated bond angles (°).

Angle	Found	Calculated	Angle	Found	Calculated
C(15)-C(16)-C(11)	120.06(11)	120.559	C(19)-C(18)-C(17)	119.81(13)	120.280
C(15)-C(16)-H(16)	122.1(9)	117.861	C(19)-C(18)-H(18)	122.1(8)	119.353
C(11)-C(16)-H(16)	117.8(9)	121.521	C(17)-C(18)-H(18)	118.1(8)	120.367
C(16)-C(11)-C(12)	119.30(10)	119.904	C(21)-C(20)-C(19)	120.16(12)	120.082
C(16)-C(11)-N(10)	124.81(10)	125.107	C(21)-C(20)-H(20)	120.4(14)	119.909
C(12)-C(11)-N(10)	115.73(9)	114.919	C(19)-C(20)-H(20)	119.3(14)	120.008
C(1)-N(10)-C(11)	131.00(9)	134.273	C(17)-C(22)-C(21)	119.69(12)	120.241
C(1)-N(10)-H(10)	113.1(9)	114.008	C(17)-C(22)-H(22)	119.4(9)	120.388
C(11)-N(10)-H(10)	115.9(9)	111.715	C(21)-C(22)-H(22)	121.0(9)	119.351
C(14)-C(13)-C(12)	119.91(11)	121.484	C(7)-C(8)-C(9)	120.1(2)	120.323
C(14)-C(13)-H(13)	121.7(9)	119.220	C(7)-C(8)-H(8)	120(2)	120.323
C(12)-C(13)-H(13)	118.3(9)	119.297	C(9)-C(8)-H(8)	120(2)	119.912
N(10)-C(1)-C(2)	121.32(9)	119.961	C(20)-C(19)-C(18)	120.26(13)	119.921
N(10)-C(1)-C(17)	119.86(9)	122.187	C(20)-C(19)-H(19)	121.4(10)	120.220
C(2)-C(1)-C(17)	118.72(9)	117.783	C(18)-C(19)-H(19)	118.3(10)	119.856
C(5)-C(4)-C(9)	119.08(12)	118.858	C(15)-C(14)-C(13)	120.21(11)	119.629
C(5)-C(4)-C(3)	118.99(11)	118.951	C(15)-C(14)-H(14)	120.7(8)	120.113
C(9)-C(4)-C(3)	121.89(11)	122.189	C(13)-C(14)-H(14)	119.1(8)	120.245
O(2)-C(12)-C(13)	124.31(10)	120.178	C(20)-C(21)-C(22)	120.31(13)	119.940
O(2)-C(12)-C(11)	115.56(9)	121.222	C(20)-C(21)-H(21)	121.7(9)	120.150
C(13)-C(12)-C(11)	120.13(10)	118.589	C(22)-C(21)-H(21)	117.9(9)	119.911
O(1)-C(3)-C(2)	122.40(9)	121.748	C(8)-C(9)-C(4)	120.4(2)	120.402
O(1)-C(3)-C(4)	117.87(9)	119.734	C(8)-C(9)-H(9)	119.7(9)	117.732
C(2)-C(3)-C(4)	119.73(9)	118.500	C(4)-C(9)-H(9)	119.5(9)	121.837
C(12)-O(2)-H(211)	113.3(11)	107.732	C(8)-C(7)-C(6)	120.35(14)	119.687
C(1)-C(2)-C(3)	123.71(10)	123.166	C(8)-C(7)-H(7)	118.1(14)	120.164
C(1)-C(2)-H(2)	117.6(7)	117.790	C(6)-C(7)-H(7)	121.5(14)	120.147
C(3)-C(2)-H(2)	118.7(7)	119.045	C(4)-C(5)-C(6)	119.4(2)	120.629
C(22)-C(17)-C(18)	119.74(10)	119.484	C(4)-C(5)-H(5)	119.5(9)	120.862
C(22)-C(17)-C(1)	121.01(10)	120.568	C(6)-C(5)-H(5)	121.1(9)	118.510
C(18)-C(17)-C(1)	119.17(10)	119.884	C(7)-C(6)-C(5)	120.6(2)	120.098
C(14)-C(15)-C(16)	120.37(11)	119.781	C(7)-C(6)-H(6)	126.0(12)	119.842
C(14)-C(15)-H(15)	125.9(9)	120.010	C(5)-C(6)-H(6)	113.3(13)	120.061
C(16)-C(15)-H(15)	113.5(9)	120.194			

**Figure 4.** ORTEP diagram of the plane (110).**Figure 5.** ORTEP diagram of the plane (111).

**Table 5.** The calculated Steric energy (kcal/mol) for the synthesized Schiff base and its tautomerisms using force field MM2 method.

Energy	L (Keto-Enol)	L	L (amine-imine)
Stretch	1.026	0.752	0.667
Bend	7.008	3.924	4.824
Stretch-bend	-0.079	0.046	0.045
Torsion	-14.335	-7.568	-10.113
Non-1.4VDW	-6.930	-6.536	-5.033
1.4VDW	11.432	12.956	10.651
Dipole-dipole	-1.781	-0.672	-1.375
Total energy	3.660	2.902	0.332

**Figure 6.** The view of the prepared single crystal.**Figure 7.** The conformation of (L) compound after energy minimization.**Scheme 1.** Keto-enol and amine-imine resonance for the L compound.

Also, the absolute value of the total energy was 3.660, 2.902 and 0.332 kcal/mol for L-keto-enol, L-compound and L-amine-imine, respectively. The steric energy value reveal that, the L-amine-imine compound is the most stable tautomer which is more favorable one which could be have the largest product %. The obtained result goes well with the single crystal analysis data. Generally, the order of the formed tautomer as L-amine-imine  $\geq$  L-compound  $>$  L-keto-enol (Scheme 1).

The formation of the intra-hydrogen bond was calculated for different conformations derived from the most stable L-amine-imine tautomer. The most stable hydrogen bond was formed due to the interaction of O(1) with H(2'). The formed bond has length equal 2.099 Å and the absolute total energy of the formed conformation equal 0.521 kcal/mol. Also, the hydrogen bond which formed due to the interaction of O(1) with H(10) has bond length = 1.66 Å and total steric energy = 0.529 kcal/ mol. The two conformations nearly have the same steric effect meanwhile the bond length for the second conformation (1.66 Å) reveal it is more stable than the first conformation [19].

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## Supporting information

CCDC 883173 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge at <http://www.ccdc.cam.ac.uk/const/retrieving.html> or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44-1223-336033 or email: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk).

## Disclosure statement

Conflict of interests: The authors declare that they have no conflict of interest.

Author contributions: All authors contributed equally to this work.

Ethical approval: All ethical guidelines have been adhered.

Sample availability: Samples of the compounds are available from the author.

ORCID 

Adel Sayed Orabi

 <http://orcid.org/0000-0003-3171-130x>

Sahar Said El-Sakka

 <http://orcid.org/0000-0003-0386-1415>

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