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(*E*)-1-[4-(2,4-Dihydroxybenzylideneamino)phenyl]ethanone sesquihydrate

Arzu Özek,[a]* Çiğdem Albayrak,[b] Mustafa Odabaşoğlu[b] and Orhan Büyükgüngör[a]

[a]Department of Physics, Ondokuz Mayıs University, TR-55139 Samsun, Turkey, and [b]Department of Chemistry, Ondokuz Mayıs University, TR-55139 Samsun, Turkey
Correspondence e-mail: arzuozek@omu.edu.tr

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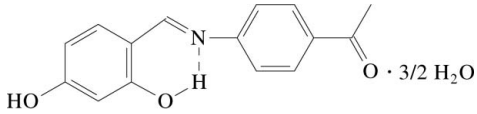
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.043; wR factor = 0.108; data-to-parameter ratio = 13.3.

The asymmetric unit of the title compound, $C_{15}H_{13}NO_3\cdot 1.5H_2O$, consists of one ethanone molecule, one water molecule and one half-molecule of water. The organic molecule is a phenol–imine tautomer, as evidenced from C—O, C—N and C—C bond lengths and it is stabilized by an intramolecular O—H···N hydrogen bond which generates an S(6) ring motif. It is nearly planar, with a dihedral angle of 1.40 (10)° between the two aromatic rings. Molecules are linked by three intermolecular O—H···O hydrogen bonds, forming dimers, and are further linked by C—H···π interactions, forming a three-dimensional network.

Related literature

For related literature, see: Elerman *et al.*, 1995; Özek *et al.*, 2007; Albayrak *et al.*, 2005; Odabaşoğlu *et al.* (2005); Odabaşoğlu *et al.* (2007*a*,*b*).



Experimental

Crystal data

$C_{15}H_{13}NO_3\cdot 1.5H_2O$
M_r = 282.29
Triclinic, $P\overline{1}$
a = 5.9812 (7) Å
b = 7.3117 (10) Å
c = 16.450 (2) Å
α = 101.031 (10)°
β = 90.948 (10)°
γ = 103.984 (10)°
V = 683.68 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.47 × 0.28 × 0.05 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.972, T_{max} = 0.996
10420 measured reflections
2675 independent reflections
1351 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.108
S = 0.87
2675 reflections
201 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*A*···O4	0.82	1.92	2.740 (2)	173
O1—H1···N1	0.82	1.87	2.608 (2)	148
O4—H4*B*···O3^{i}	0.860 (16)	1.931 (17)	2.787 (2)	173 (3)
O4—H4*A*···O4^{ii}	0.760 (16)	2.108 (16)	2.848 (4)	165 (4)
C14—H14a···*Cg*1^{iii}	0.96	2.78	3.590 (2)	143

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2057).

References

Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005). *Acta Cryst.* E**61**, o423–o424.
Elerman, Y., Elmali, A. & Svoboda, I. (1995). *Acta Cryst.* C**51**, 2344–2346.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2005). *Acta Cryst.* E**61**, o425–o426.
Odabaşoğlu, M., Arslan, F., Ölmez, H. & Büyükgüngör, O. (2007*a*). *Acta Cryst.* E**63**, o3654.
Odabaşoğlu, M., Büyükgüngör, O., Narayana, B., Vijeshi, A. M. & Yathirajan, H. S. (2007*b*). *Acta Cryst.* E**63**, o1916–o1918.
Özek, A., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2007). *Acta Cryst.* C**63**, o177–o180.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

supplementary materials

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(*E*)-1-[4-(2,4-Dihydroxybenzylideneamino)phenyl]ethanone sesquihydrate

A. Özek, Ç. Albayrak, M. Odabasoglu and O. Büyükgüngör

Comment

The present work is part of a structural study of Schiff bases Özek *et al.*, 2007; Odabaşoğlu *et al.*, 2007*a*,b) and we report here the structure of (*E*)-1-(4-(2,4-dihydroxybenzylideneamino)phenyl)ethanone. 3/2 hydrate, (I).

In general, *O*-hydroxy Schiff bases exhibit two possible tautomeric forms, the phenol-imine (or benzenoid) and keto-amine (or quinoid) forms. Depending on the tautomers, two types of intra-molecular hydrogen bonds are possible: O—H···N in benzenoid and N—H···O in quinoid tautomers. The H atom in title compound (I) is located on atom O1, thus the phenol-imine tautomer is favored over the keto-amine form, as indicated by the C6—O1, C7—N1, C1—C7 and C1—C6 bond lengths (Fig. 1 and Table 1). The O1—C6 bond length of 1.346 (2) Å indicates single-bond character, whereas the N1—C7 bond length of 1.287 (2) Å indicates a high degree of double-bond character. A similar work was observed for 2-(3-Methoxysalicylideneamino)-1*H*-benzimidazolemonohydrate [C—O=1.357 (2) Å, C—N= 1.285 (2) Å, Albayrak *et al.*, 2005]. It is known that Schiff bases may exhibit thermochromism or photochromism, depending on the planarity or non-planarity of the molecule, respectively. Therefore, one can expect thermochromic properties in (I) caused by planarity of the molecules; the dihedral angle between rings A(C1—C6) and B ring (C8—C13) is 1.4 °. Fig.1 shows an intramolecular O1—H1···N1 hydrogen bond that generates an S(6) ring motif. The O1···N1 distance of 2.608 (2) Å is comparable to those observed for analogous hydrogen bonds in *N*-(2-hydroxyphenyl)salicylaldimine [2.675 (7) Å; Elerman *et al.*, 1995] and Three (*E*)-2-[(bromophenyl)iminomethyl]-4-methoxyphenols [2.603 (2) Å, 2.638 (7) Å, 2.577 (4) Å;Özek *et al.*, 2007]. In the crystal structure of (I), the molecules are linked by three O—H···O intermolecular hydrogen bonds (Fig.2) and further linked by C—H···π interactions (Table 2), forming a three-dimensional network.

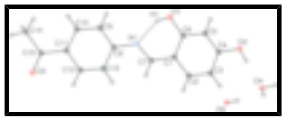
Experimental

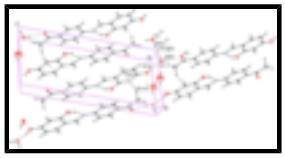
The title compounds were prepared as described by (Odabaşoğlu *et al.*, 2005), 4-acetylaniline and 4-hydroxysalicylaldehyde as starting materials. Well shaped crystals of (I) were obtained by slow evaporation of an ethyl alcohol solution [(I): yield 76%; m.p. 447–449 K].

Refinement

The coordinates of the H atoms of the water molecules were located in the difference Fourier map and were then allowed to refine subject to a restraint of the distance O—H = 0.82 Å. All other H atoms were refined using a riding model, with C—H distance of 0.93Å for aromatic H atoms and 0.96Å for methyl H atoms, O—H distances of 0.82 Å, and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C,*O*) for the remaining H atoms.

Figures





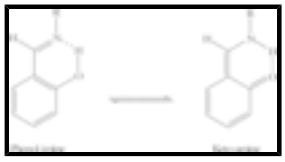


Figure 1. An *ORTEP* view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. Dashed line indicates intramolecular hydrogen bond.
Figure 2. A partial packing view of (I), showing the formation of the intermolecular hydrogen bonds and C—H···π interactions. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code; (i): $1-x, y-1/2, 1-z$; (ii): $-x, -y, -z$]

(*E*)-1-[4-(2,4-Dihydroxybenzylideneamino)phenyl]ethanone sesquihydrate

Crystal data

$C_{15}H_{13}NO_3 \cdot 1.5H_2O$	$Z = 2$
$M_r = 282.29$	$F_{000} = 298$
Triclinic, $P\overline{1}$	$D_x = 1.366$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.9812$ (7) Å	Cell parameters from 10420 reflections
$b = 7.3117$ (10) Å	$\theta = 2.5$–29.4º
$c = 16.450$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 101.031$ (10)º	$T = 296$ K
$\beta = 90.948$ (10)º	Plate, yellow
$\gamma = 103.984$ (10)º	0.47 × 0.28 × 0.05 mm
$V = 683.68$ (15) Å^3	

Data collection

Stoe IPDS-2 diffractometer	2675 independent reflections
Radiation source: fine-focus sealed tube	1351 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.084$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 296$ K	$\theta_{min} = 2.5$º
ω scans	$h = -7 \rightarrow 7$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$k = -8 \rightarrow 9$
$T_{min} = 0.972$, $T_{max} = 0.996$	$l = -20 \rightarrow 20$
10420 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.87$	$(\Delta/\sigma)_{max} < 0.001$
2675 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
201 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. 390 frames, detector distance = 100 mm

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.4432 (3)	0.5425 (3)	0.30698 (11)	0.0430 (5)	
C2	0.2610 (3)	0.4313 (3)	0.25090 (11)	0.0509 (5)	
H2	0.1124	0.4050	0.2692	0.061*	
C3	0.2932 (3)	0.3603 (3)	0.17049 (12)	0.0551 (6)	
H3	0.1686	0.2871	0.1344	0.066*	
C4	0.5149 (3)	0.3986 (3)	0.14294 (12)	0.0503 (5)	
C5	0.6998 (3)	0.5072 (3)	0.19635 (12)	0.0545 (5)	
H5	0.8473	0.5332	0.1772	0.065*	
C6	0.6665 (3)	0.5773 (3)	0.27794 (11)	0.0459 (5)	
C7	0.4009 (3)	0.6152 (3)	0.39078 (11)	0.0481 (5)	
H7	0.2496	0.5897	0.4065	0.058*	
C8	0.5185 (3)	0.7859 (3)	0.52783 (11)	0.0426 (5)	
C9	0.7081 (3)	0.8923 (3)	0.58016 (11)	0.0510 (5)	
H9	0.8541	0.9144	0.5597	0.061*	
C10	0.6836 (3)	0.9658 (3)	0.66222 (12)	0.0510 (5)	

H10	0.8135	1.0352	0.6965	0.061*	
C11	0.4683 (3)	0.9379 (3)	0.69432 (10)	0.0427 (5)	
C12	0.2788 (3)	0.8344 (3)	0.64127 (12)	0.0528 (5)	
H12	0.1324	0.8154	0.6614	0.063*	
C13	0.3019 (3)	0.7593 (3)	0.55983 (12)	0.0554 (6)	
H13	0.1717	0.6899	0.5257	0.067*	
C14	0.6365 (4)	1.1200 (3)	0.84147 (13)	0.0641 (6)	
H14A	0.6803	1.2521	0.8360	0.096*	
H14B	0.7634	1.0625	0.8290	0.096*	
H14C	0.5961	1.1135	0.8973	0.096*	
C15	0.4330 (3)	1.0136 (3)	0.78228 (12)	0.0482 (5)	
N1	0.5631 (3)	0.7144 (2)	0.44546 (9)	0.0456 (4)	
O2	0.5554 (2)	0.3308 (2)	0.06343 (8)	0.0715 (5)	
H2A	0.4333	0.2690	0.0378	0.107*	
O1	0.8501 (2)	0.6808 (2)	0.32915 (8)	0.0659 (5)	
H1	0.8074	0.7135	0.3756	0.099*	
O3	0.2375 (3)	0.9894 (2)	0.80607 (8)	0.0663 (4)	
O4	0.1563 (3)	0.1450 (3)	−0.03210 (10)	0.0806 (6)	
H4A	0.090 (5)	0.056 (4)	−0.0173 (19)	0.121*	
H4B	0.192 (5)	0.103 (4)	−0.0814 (12)	0.121*	
O5	−0.026 (7)	0.505 (5)	0.0116 (19)	0.139 (5)	0.50
H5O	0.005 (6)	0.405 (4)	−0.009 (2)	0.050 (9)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0447 (10)	0.0441 (12)	0.0389 (10)	0.0115 (9)	0.0035 (8)	0.0049 (9)
C2	0.0413 (10)	0.0607 (14)	0.0453 (11)	0.0075 (10)	0.0019 (8)	0.0041 (10)
C3	0.0500 (12)	0.0623 (15)	0.0448 (11)	0.0081 (11)	−0.0046 (9)	−0.0015 (10)
C4	0.0562 (12)	0.0531 (13)	0.0391 (10)	0.0146 (10)	0.0039 (9)	0.0017 (9)
C5	0.0459 (11)	0.0654 (15)	0.0479 (11)	0.0123 (11)	0.0080 (9)	0.0025 (10)
C6	0.0387 (10)	0.0489 (13)	0.0456 (11)	0.0077 (9)	−0.0001 (8)	0.0028 (9)
C7	0.0430 (10)	0.0551 (14)	0.0451 (11)	0.0121 (10)	0.0047 (9)	0.0074 (10)
C8	0.0452 (10)	0.0431 (12)	0.0391 (10)	0.0119 (9)	0.0022 (8)	0.0064 (9)
C9	0.0398 (10)	0.0640 (15)	0.0452 (11)	0.0089 (10)	0.0037 (8)	0.0064 (10)
C10	0.0434 (11)	0.0597 (14)	0.0429 (11)	0.0057 (10)	−0.0021 (8)	0.0028 (10)
C11	0.0482 (11)	0.0425 (12)	0.0368 (10)	0.0108 (9)	0.0010 (8)	0.0069 (9)
C12	0.0406 (10)	0.0662 (15)	0.0451 (11)	0.0070 (10)	0.0071 (8)	0.0030 (10)
C13	0.0428 (11)	0.0685 (16)	0.0444 (11)	0.0037 (11)	0.0010 (9)	−0.0012 (10)
C14	0.0689 (14)	0.0687 (16)	0.0443 (11)	0.0107 (12)	−0.0055 (10)	−0.0051 (10)
C15	0.0557 (12)	0.0458 (13)	0.0420 (10)	0.0119 (10)	0.0027 (9)	0.0070 (9)
N1	0.0464 (9)	0.0490 (11)	0.0395 (8)	0.0128 (8)	0.0026 (7)	0.0031 (7)
O2	0.0660 (9)	0.0953 (12)	0.0411 (8)	0.0151 (9)	0.0065 (7)	−0.0096 (8)
O1	0.0431 (7)	0.0862 (12)	0.0504 (8)	0.0025 (7)	0.0012 (6)	−0.0122 (7)
O3	0.0608 (9)	0.0832 (12)	0.0456 (8)	0.0106 (8)	0.0116 (7)	−0.0013 (7)
O4	0.0796 (12)	0.1020 (15)	0.0457 (9)	0.0092 (11)	0.0095 (8)	−0.0041 (9)
O5	0.165 (15)	0.169 (7)	0.103 (14)	0.101 (8)	0.010 (9)	0.001 (9)

Geometric parameters (Å, °)

C1—C2	1.397 (3)	C10—C11	1.384 (3)
C1—C6	1.407 (2)	C10—H10	0.9300
C1—C7	1.429 (3)	C11—C12	1.385 (3)
C2—C3	1.360 (3)	C11—C15	1.485 (3)
C2—H2	0.9300	C12—C13	1.370 (3)
C3—C4	1.389 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—H13	0.9300
C4—O2	1.355 (2)	C14—C15	1.499 (3)
C4—C5	1.379 (3)	C14—H14A	0.9600
C5—C6	1.378 (3)	C14—H14B	0.9600
C5—H5	0.9300	C14—H14C	0.9600
C6—O1	1.346 (2)	C15—O3	1.222 (2)
C7—N1	1.287 (2)	O2—H2A	0.8200
C7—H7	0.9300	O1—H1	0.8200
C8—C9	1.385 (2)	O4—H4A	0.760 (16)
C8—C13	1.390 (3)	O4—H4B	0.860 (16)
C8—N1	1.410 (2)	O5—O5^{i}	0.50 (4)
C9—C10	1.378 (3)	O5—H5O	0.81 (2)
C9—H9	0.9300		
C2—C1—C6	117.59 (16)	C9—C10—C11	120.94 (17)
C2—C1—C7	120.31 (17)	C9—C10—H10	119.5
C6—C1—C7	122.10 (17)	C11—C10—H10	119.5
C3—C2—C1	122.27 (18)	C10—C11—C12	117.84 (17)
C3—C2—H2	118.9	C10—C11—C15	122.98 (17)
C1—C2—H2	118.9	C12—C11—C15	119.18 (17)
C2—C3—C4	119.11 (18)	C13—C12—C11	121.60 (18)
C2—C3—H3	120.4	C13—C12—H12	119.2
C4—C3—H3	120.4	C11—C12—H12	119.2
O2—C4—C5	118.32 (19)	C12—C13—C8	120.51 (18)
O2—C4—C3	121.20 (18)	C12—C13—H13	119.7
C5—C4—C3	120.48 (18)	C8—C13—H13	119.7
C6—C5—C4	120.21 (18)	C15—C14—H14A	109.5
C6—C5—H5	119.9	C15—C14—H14B	109.5
C4—C5—H5	119.9	H14A—C14—H14B	109.5
O1—C6—C5	119.11 (16)	C15—C14—H14C	109.5
O1—C6—C1	120.56 (16)	H14A—C14—H14C	109.5
C5—C6—C1	120.33 (16)	H14B—C14—H14C	109.5
N1—C7—C1	122.84 (18)	O3—C15—C11	119.72 (17)
N1—C7—H7	118.6	O3—C15—C14	120.24 (19)
C1—C7—H7	118.6	C11—C15—C14	120.04 (18)
C9—C8—C13	118.16 (17)	C7—N1—C8	122.20 (16)
C9—C8—N1	116.39 (17)	C4—O2—H2A	109.5
C13—C8—N1	125.45 (17)	C6—O1—H1	109.5
C10—C9—C8	120.93 (18)	H4A—O4—H4B	105 (2)
C10—C9—H9	119.5	O5^{i}—O5—H5O	53 (7)

C8—C9—H9	119.5		
C6—C1—C2—C3	−1.1 (3)	N1—C8—C9—C10	−178.88 (19)
C7—C1—C2—C3	179.6 (2)	C8—C9—C10—C11	−1.0 (3)
C1—C2—C3—C4	0.2 (3)	C9—C10—C11—C12	−0.2 (3)
C2—C3—C4—O2	180.0 (2)	C9—C10—C11—C15	179.8 (2)
C2—C3—C4—C5	0.0 (3)	C10—C11—C12—C13	0.8 (3)
O2—C4—C5—C6	−179.3 (2)	C15—C11—C12—C13	−179.2 (2)
C3—C4—C5—C6	0.6 (3)	C11—C12—C13—C8	−0.3 (3)
C4—C5—C6—O1	179.2 (2)	C9—C8—C13—C12	−0.9 (3)
C4—C5—C6—C1	−1.5 (3)	N1—C8—C13—C12	179.5 (2)
C2—C1—C6—O1	−178.99 (19)	C10—C11—C15—O3	177.6 (2)
C7—C1—C6—O1	0.4 (3)	C12—C11—C15—O3	−2.4 (3)
C2—C1—C6—C5	1.7 (3)	C10—C11—C15—C14	−2.2 (3)
C7—C1—C6—C5	−179.00 (19)	C12—C11—C15—C14	177.8 (2)
C2—C1—C7—N1	178.31 (19)	C1—C7—N1—C8	179.68 (19)
C6—C1—C7—N1	−1.0 (3)	C9—C8—N1—C7	−179.31 (18)
C13—C8—C9—C10	1.5 (3)	C13—C8—N1—C7	0.3 (3)

Symmetry codes: (i) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O4	0.82	1.92	2.740 (2)	173
O1—H1···N1	0.82	1.87	2.608 (2)	148
O4—H4B···O3^{ii}	0.860 (16)	1.931 (17)	2.787 (2)	173 (3)
O4—H4A···O4^{iii}	0.760 (16)	2.108 (16)	2.848 (4)	165 (4)
C14—H14a···Cg1^{iv}	0.96	2.779	3.590 (2)	143

Symmetry codes: (ii) *x*, *y*−1, *z*−1; (iii) −*x*, −*y*, −*z*; (iv) −*x*+1, −*y*+2, −*z*+1.

Fig. 1

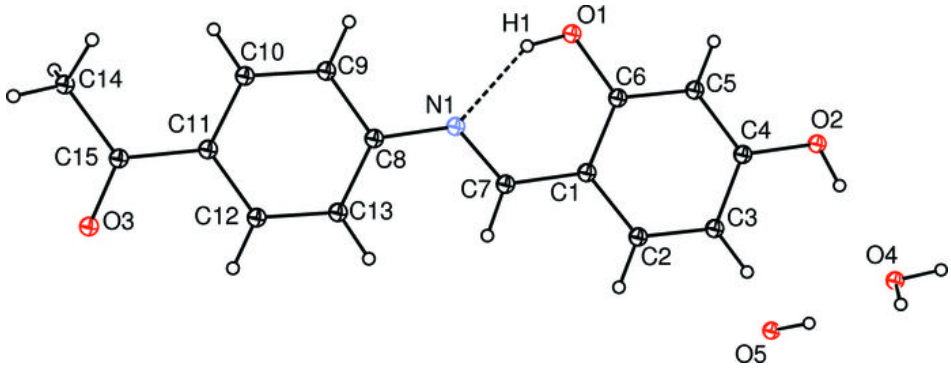

H1
O1
C10
C9
C14
C6
C5
N1
C11
C4
O2
C15
C8
C7
C1
O3
C12
C13
C3
C2
O4
O5

Fig. 2

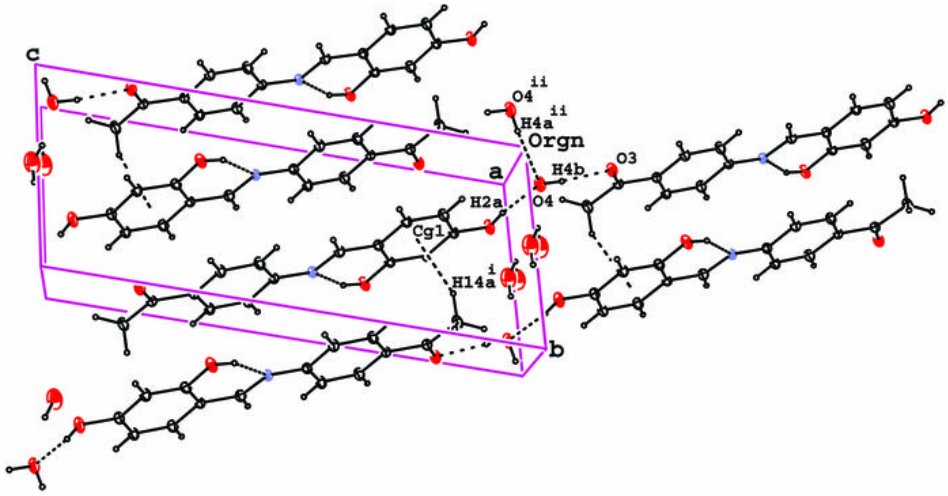
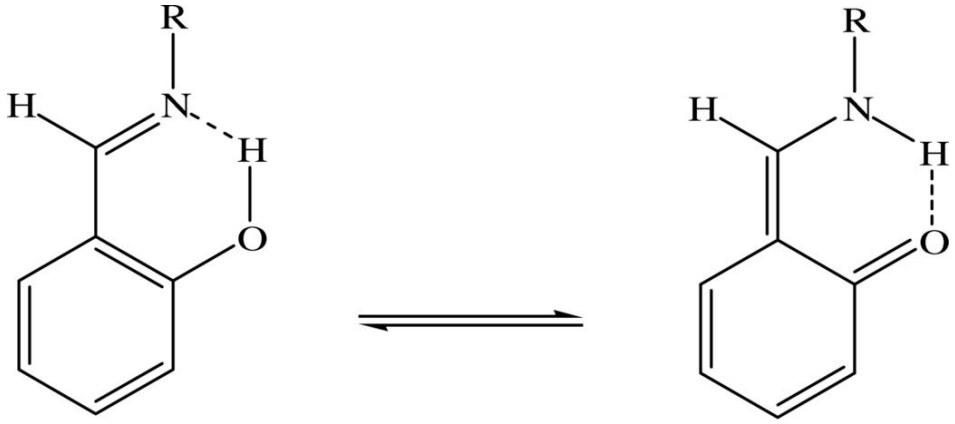


Fig. 3



Phenol-imine Keto-amine