

(2,4-Dimethoxybenzylidene)-2-hydroxybenzohydrazide ethanol solvate

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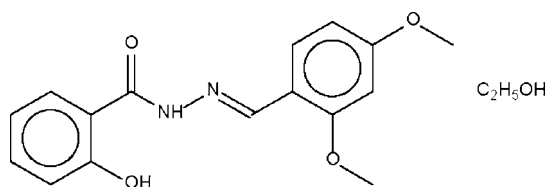
Received 22 April 2008; accepted 24 April 2008

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
R factor = 0.047; wR factor = 0.118; data-to-parameter ratio = 16.0.

In the planar title molecule, $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_4 \cdot \text{C}_2\text{H}_6\text{O}$, the planar Schiff base molecule is linked to the ethanol solvent molecule by a hydroxy–amide hydrogen bond. The hydroxy group of the ethanol molecule is a hydrogen-bond donor to the double-bonded N atom of an adjacent Schiff base, pairs of interactions taking place across a center of symmetry and giving rise to a hydrogen-bonded dimer.

Related literature

For the crystal structures of other substituted benzylidene-2-hydroxybenzohydrazides, see: Li (2007); Liang *et al.* (2005); Luo (2007); Ma *et al.* (2005); Pan & Yang (2005*a,b,c*); Qiu *et al.* (2006); Shao *et al.* (2004); Wang *et al.* (2007); Xu & Liu (2006); Yang (2006); Yang & Pan (2004, 2005*a,b*); Zhang *et al.* (2006).

**Experimental***Crystal data*

$\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_4 \cdot \text{C}_2\text{H}_6\text{O}$
 $M_r = 346.38$
 Monoclinic, $P2_1/n$
 $a = 7.7909$ (2) Å
 $b = 18.0539$ (6) Å
 $c = 12.0001$ (4) Å
 $\beta = 93.803$ (2)°

$V = 1684.17$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 100$ (2) K
 $0.20 \times 0.15 \times 0.15$ mm

Data collection

Bruker SMART APEX
 diffractometer
 Absorption correction: none
 13796 measured reflections

3853 independent reflections
 2575 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.118$
 $S = 1.03$
 3853 reflections
 241 parameters
 3 restraints

H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1–H1o \cdots O2	0.86 (1)	1.74 (2)	2.528 (2)	151 (2)
O5–H5o \cdots N2 ⁱ	0.85 (1)	2.07 (1)	2.847 (2)	152 (2)
N1–H1n \cdots O5	0.86 (1)	2.09 (1)	2.894 (2)	157 (2)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

We acknowledge the SAGA grant (06–02–03–0147) for support of this study, and the University of Malaya for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2239).

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supplementary materials

Acta Cryst. (2008). E64, o961 [doi:10.1107/S1600536808011768]

(2,4-Dimethoxybenzylidene)-2-hydroxybenzohydrazide ethanol solvate

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Comment

The crystal structures of a number of substituted benzylidene-2-hydroxybenzohydrazides have been reported (Li, 2007; Liang *et al.*, 2005; Luo, 2007; Ma *et al.*, 2005; Pan & Yang, 2005*a,b,c*; Qiu *et al.*, 2006; Shao *et al.*, 2004; Wang *et al.*, 2007; Xu & Liu, 2006; Yang, 2006; Yang & Pan, 2004, 2005*a,b*; Zhang *et al.*, 2006).

The 2,4-dimethoxy derivative crystallizes as an ethanol solvate (Scheme I, Fig. 1). The planar molecule of $C_{16}H_{16}N_2O_4$ is linked to the ethanol molecule by an amido \cdots hydroxy_{ethanol} hydrogen bond [N–H \cdots O 2.894 (2) Å]. The hydroxy unit of the ethanol molecule is a hydrogen-bond donor site to the double-bond nitrogen atom of an adjacent Schiff base [O–H \cdots N 2.847 (2) Å], this interaction across a center of symmetry giving rise to a hydrogen-bonded dimer (Fig. 2).

Experimental

2-Hydroxybenzohydrazide (0.60 g, 4 mmol) and 2,4-dimethoxybenzaldehyde (0.66 g, 4 mmol) were heated in ethanol (30 ml) for 2 h. The solvent was removed by evaporation and the product recrystallized from ethanol.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2–1.5 $U(C)$.

The oxygen- and nitrogen-bound H-atoms were located in a difference Fourier map, and were refined with a distance restraint (O–H = N–H 0.85 Å); their temperature factors were freely refined.

Figures

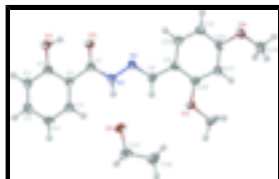


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{16}H_{16}N_2O_4 \cdot C_2H_6O$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radii.

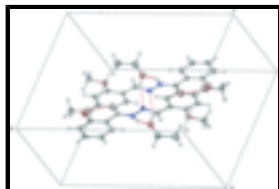


Fig. 2. Hydrogen-bonded dimeric structure.

(2,4-Dimethoxybenzylidene)-2-hydroxybenzohydrazide ethanol solvate

Crystal data

C₁₆H₁₆N₂O₄·C₂H₆O

M_r = 346.38

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2₁ *n*

a = 7.7909 (2) Å

b = 18.0539 (6) Å

c = 12.0001 (4) Å

β = 93.803 (2)°

V = 1684.17 (9) Å³

Z = 4

*F*₀₀₀ = 736

D_x = 1.366 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 1895 reflections

θ = 2.8–25.5°

μ = 0.10 mm⁻¹

T = 100 (2) K

Prism, colorless

0.20 × 0.15 × 0.15 mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 100(2) K

ω scans

Absorption correction: None

13796 measured reflections

3853 independent reflections

2575 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.059

θ_{max} = 27.5°

θ_{min} = 2.0°

h = -10→10

k = -20→23

l = -15→15

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.046

wR(*F*²) = 0.118

S = 1.03

3853 reflections

241 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.175P]$$

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 0.21 e Å⁻³

Δρ_{min} = -0.24 e Å⁻³

Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.64682 (15)	0.22307 (7)	0.69448 (11)	0.0248 (3)
O2	0.48542 (15)	0.30514 (7)	0.55256 (10)	0.0253 (3)
O3	0.09164 (14)	0.62457 (7)	0.44328 (10)	0.0224 (3)
O4	-0.15888 (16)	0.55131 (7)	0.07909 (10)	0.0280 (3)
O5	0.45339 (16)	0.56902 (7)	0.68732 (11)	0.0256 (3)
N1	0.40917 (17)	0.42200 (9)	0.59366 (12)	0.0191 (3)
N2	0.32044 (17)	0.42928 (8)	0.48948 (11)	0.0195 (3)
C1	0.6546 (2)	0.28297 (10)	0.76338 (14)	0.0199 (4)
C2	0.7381 (2)	0.27412 (10)	0.86870 (14)	0.0219 (4)
H2	0.7858	0.2275	0.8904	0.026*
C3	0.7514 (2)	0.33316 (11)	0.94120 (14)	0.0231 (4)
H3	0.8073	0.3266	1.0133	0.028*
C4	0.6847 (2)	0.40220 (10)	0.91101 (14)	0.0230 (4)
H4	0.6962	0.4428	0.9614	0.028*
C5	0.6014 (2)	0.41094 (10)	0.80671 (14)	0.0211 (4)
H5	0.5560	0.4581	0.7856	0.025*
C6	0.5825 (2)	0.35172 (10)	0.73132 (14)	0.0180 (4)
C7	0.4908 (2)	0.35796 (10)	0.61929 (14)	0.0192 (4)
C8	0.22902 (19)	0.48872 (10)	0.47864 (14)	0.0188 (4)
H8	0.2277	0.5226	0.5391	0.023*
C9	0.1282 (2)	0.50446 (10)	0.37526 (14)	0.0185 (4)
C10	0.0552 (2)	0.57510 (10)	0.35888 (14)	0.0189 (4)
C11	-0.0433 (2)	0.59274 (10)	0.26156 (14)	0.0197 (4)
H11	-0.0930	0.6405	0.2519	0.024*
C12	-0.0677 (2)	0.53942 (10)	0.17899 (14)	0.0213 (4)
C13	0.0016 (2)	0.46857 (10)	0.19353 (15)	0.0227 (4)
H13	-0.0173	0.4321	0.1369	0.027*
C14	0.0973 (2)	0.45200 (10)	0.29057 (14)	0.0205 (4)
H14	0.1438	0.4036	0.3004	0.025*
C15	0.0125 (2)	0.69592 (10)	0.43449 (15)	0.0240 (4)
H15A	0.0456	0.7250	0.5015	0.036*
H15B	-0.1128	0.6902	0.4275	0.036*
H15C	0.0505	0.7215	0.3685	0.036*
C16	-0.2167 (2)	0.62483 (11)	0.05390 (16)	0.0281 (4)
H16A	-0.2707	0.6264	-0.0222	0.042*
H16B	-0.1184	0.6588	0.0597	0.042*
H16C	-0.3006	0.6398	0.1069	0.042*
C17	0.4115 (2)	0.62589 (11)	0.76362 (15)	0.0278 (4)
H17A	0.5186	0.6506	0.7929	0.033*
H17B	0.3567	0.6033	0.8275	0.033*
C18	0.2921 (2)	0.68255 (11)	0.70951 (16)	0.0310 (5)
H18A	0.2608	0.7187	0.7655	0.046*
H18B	0.1881	0.6579	0.6775	0.046*
H18C	0.3496	0.7079	0.6502	0.046*
H1O	0.594 (3)	0.2375 (13)	0.6331 (12)	0.054 (7)*

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H5O	0.518 (2)	0.5858 (13)	0.6389 (15)	0.052 (7)*
H1N	0.410 (3)	0.4596 (8)	0.6371 (14)	0.036 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0311 (7)	0.0185 (7)	0.0241 (7)	0.0015 (5)	-0.0021 (6)	-0.0001 (6)
O2	0.0328 (7)	0.0185 (7)	0.0236 (7)	0.0024 (5)	-0.0045 (5)	-0.0035 (6)
O3	0.0291 (6)	0.0170 (7)	0.0208 (7)	0.0034 (5)	-0.0009 (5)	-0.0022 (5)
O4	0.0342 (7)	0.0261 (8)	0.0225 (7)	0.0032 (6)	-0.0077 (5)	0.0004 (6)
O5	0.0313 (7)	0.0212 (7)	0.0247 (7)	0.0003 (6)	0.0063 (6)	-0.0036 (6)
N1	0.0227 (7)	0.0181 (8)	0.0163 (8)	-0.0002 (6)	-0.0007 (6)	-0.0006 (7)
N2	0.0206 (7)	0.0205 (8)	0.0169 (8)	-0.0006 (6)	-0.0012 (6)	0.0010 (7)
C1	0.0190 (8)	0.0193 (10)	0.0218 (9)	-0.0023 (7)	0.0033 (7)	-0.0003 (8)
C2	0.0212 (8)	0.0210 (10)	0.0233 (10)	0.0009 (7)	0.0000 (7)	0.0044 (8)
C3	0.0224 (8)	0.0285 (11)	0.0183 (9)	-0.0043 (8)	0.0001 (7)	0.0050 (8)
C4	0.0263 (9)	0.0235 (10)	0.0194 (9)	-0.0042 (7)	0.0031 (7)	-0.0034 (8)
C5	0.0221 (8)	0.0181 (10)	0.0232 (10)	-0.0003 (7)	0.0022 (7)	0.0017 (8)
C6	0.0192 (8)	0.0169 (10)	0.0181 (9)	-0.0020 (7)	0.0018 (6)	0.0009 (7)
C7	0.0187 (8)	0.0176 (10)	0.0214 (9)	-0.0012 (7)	0.0024 (7)	-0.0001 (8)
C8	0.0190 (8)	0.0181 (9)	0.0198 (9)	-0.0010 (7)	0.0044 (7)	0.0001 (8)
C9	0.0191 (8)	0.0187 (9)	0.0179 (9)	-0.0014 (7)	0.0032 (6)	0.0005 (8)
C10	0.0181 (8)	0.0193 (10)	0.0196 (9)	-0.0026 (7)	0.0043 (7)	-0.0026 (8)
C11	0.0195 (8)	0.0179 (10)	0.0218 (9)	0.0012 (7)	0.0027 (7)	0.0028 (8)
C12	0.0210 (8)	0.0228 (10)	0.0200 (9)	-0.0026 (7)	0.0009 (7)	0.0018 (8)
C13	0.0253 (9)	0.0206 (10)	0.0218 (10)	-0.0024 (7)	-0.0006 (7)	-0.0034 (8)
C14	0.0217 (8)	0.0158 (9)	0.0240 (10)	-0.0014 (7)	0.0023 (7)	0.0007 (8)
C15	0.0268 (9)	0.0187 (10)	0.0267 (10)	0.0036 (7)	0.0032 (7)	-0.0032 (8)
C16	0.0288 (9)	0.0294 (11)	0.0254 (10)	0.0027 (8)	-0.0031 (8)	0.0047 (9)
C17	0.0319 (10)	0.0270 (11)	0.0245 (10)	0.0004 (8)	0.0026 (8)	-0.0066 (9)
C18	0.0323 (10)	0.0270 (12)	0.0339 (11)	0.0002 (8)	0.0040 (8)	-0.0023 (9)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.360 (2)	C8—C9	1.452 (2)
O1—H1O	0.859 (9)	C8—H8	0.9500
O2—C7	1.244 (2)	C9—C14	1.398 (2)
O3—C10	1.366 (2)	C9—C10	1.405 (2)
O3—C15	1.429 (2)	C10—C11	1.391 (2)
O4—C12	1.369 (2)	C11—C12	1.385 (2)
O4—C16	1.428 (2)	C11—H11	0.9500
O5—C17	1.428 (2)	C12—C13	1.395 (2)
O5—H5O	0.848 (10)	C13—C14	1.374 (2)
N1—C7	1.345 (2)	C13—H13	0.9500
N1—N2	1.3941 (19)	C14—H14	0.9500
N1—H1N	0.855 (9)	C15—H15A	0.9800
N2—C8	1.290 (2)	C15—H15B	0.9800
C1—C2	1.392 (2)	C15—H15C	0.9800
C1—C6	1.405 (2)	C16—H16A	0.9800

C2—C3	1.375 (2)	C16—H16B	0.9800
C2—H2	0.9500	C16—H16C	0.9800
C3—C4	1.389 (3)	C17—C18	1.501 (3)
C3—H3	0.9500	C17—H17A	0.9900
C4—C5	1.380 (2)	C17—H17B	0.9900
C4—H4	0.9500	C18—H18A	0.9800
C5—C6	1.402 (2)	C18—H18B	0.9800
C5—H5	0.9500	C18—H18C	0.9800
C6—C7	1.485 (2)		
C1—O1—H1O	106.2 (16)	C11—C10—C9	121.39 (16)
C10—O3—C15	117.86 (13)	C12—C11—C10	118.89 (16)
C12—O4—C16	117.97 (14)	C12—C11—H11	120.6
C17—O5—H5O	110.7 (17)	C10—C11—H11	120.6
C7—N1—N2	119.00 (15)	O4—C12—C11	123.77 (16)
C7—N1—H1N	123.9 (14)	O4—C12—C13	115.29 (16)
N2—N1—H1N	117.1 (14)	C11—C12—C13	120.94 (16)
C8—N2—N1	113.99 (14)	C14—C13—C12	119.31 (17)
O1—C1—C2	117.39 (16)	C14—C13—H13	120.3
O1—C1—C6	122.35 (15)	C12—C13—H13	120.3
C2—C1—C6	120.27 (16)	C13—C14—C9	121.74 (17)
C3—C2—C1	119.77 (17)	C13—C14—H14	119.1
C3—C2—H2	120.1	C9—C14—H14	119.1
C1—C2—H2	120.1	O3—C15—H15A	109.5
C2—C3—C4	121.28 (16)	O3—C15—H15B	109.5
C2—C3—H3	119.4	H15A—C15—H15B	109.5
C4—C3—H3	119.4	O3—C15—H15C	109.5
C5—C4—C3	118.97 (17)	H15A—C15—H15C	109.5
C5—C4—H4	120.5	H15B—C15—H15C	109.5
C3—C4—H4	120.5	O4—C16—H16A	109.5
C4—C5—C6	121.40 (17)	O4—C16—H16B	109.5
C4—C5—H5	119.3	H16A—C16—H16B	109.5
C6—C5—H5	119.3	O4—C16—H16C	109.5
C5—C6—C1	118.29 (15)	H16A—C16—H16C	109.5
C5—C6—C7	123.38 (16)	H16B—C16—H16C	109.5
C1—C6—C7	118.32 (15)	O5—C17—C18	111.97 (15)
O2—C7—N1	121.10 (16)	O5—C17—H17A	109.2
O2—C7—C6	121.22 (15)	C18—C17—H17A	109.2
N1—C7—C6	117.66 (15)	O5—C17—H17B	109.2
N2—C8—C9	120.86 (16)	C18—C17—H17B	109.2
N2—C8—H8	119.6	H17A—C17—H17B	107.9
C9—C8—H8	119.6	C17—C18—H18A	109.5
C14—C9—C10	117.70 (15)	C17—C18—H18B	109.5
C14—C9—C8	123.06 (16)	H18A—C18—H18B	109.5
C10—C9—C8	119.23 (16)	C17—C18—H18C	109.5
O3—C10—C11	123.27 (16)	H18A—C18—H18C	109.5
O3—C10—C9	115.32 (15)	H18B—C18—H18C	109.5
C7—N1—N2—C8	171.60 (15)	N2—C8—C9—C14	12.2 (2)
O1—C1—C2—C3	179.24 (15)	N2—C8—C9—C10	-168.70 (15)

supplementary materials

C6—C1—C2—C3	-0.6 (2)	C15—O3—C10—C11	5.3 (2)
C1—C2—C3—C4	-0.8 (2)	C15—O3—C10—C9	-176.25 (14)
C2—C3—C4—C5	1.0 (2)	C14—C9—C10—O3	-178.97 (14)
C3—C4—C5—C6	0.2 (2)	C8—C9—C10—O3	1.9 (2)
C4—C5—C6—C1	-1.6 (2)	C14—C9—C10—C11	-0.5 (2)
C4—C5—C6—C7	178.61 (15)	C8—C9—C10—C11	-179.61 (15)
O1—C1—C6—C5	-178.08 (14)	O3—C10—C11—C12	177.63 (14)
C2—C1—C6—C5	1.7 (2)	C9—C10—C11—C12	-0.7 (2)
O1—C1—C6—C7	1.8 (2)	C16—O4—C12—C11	6.8 (2)
C2—C1—C6—C7	-178.44 (14)	C16—O4—C12—C13	-173.16 (15)
N2—N1—C7—O2	-1.3 (2)	C10—C11—C12—O4	-178.49 (15)
N2—N1—C7—C6	-179.38 (13)	C10—C11—C12—C13	1.5 (2)
C5—C6—C7—O2	175.88 (16)	O4—C12—C13—C14	179.01 (14)
C1—C6—C7—O2	-4.0 (2)	C11—C12—C13—C14	-0.9 (3)
C5—C6—C7—N1	-6.1 (2)	C12—C13—C14—C9	-0.3 (3)
C1—C6—C7—N1	174.10 (15)	C10—C9—C14—C13	1.0 (2)
N1—N2—C8—C9	-179.75 (14)	C8—C9—C14—C13	-179.89 (15)

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1o \cdots O2	0.86 (1)	1.74 (2)	2.528 (2)	151 (2)
O5—H5o \cdots N2 ⁱ	0.85 (1)	2.07 (1)	2.847 (2)	152 (2)
N1—H1n \cdots O5	0.86 (1)	2.09 (1)	2.894 (2)	157 (2)

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

Fig. 1

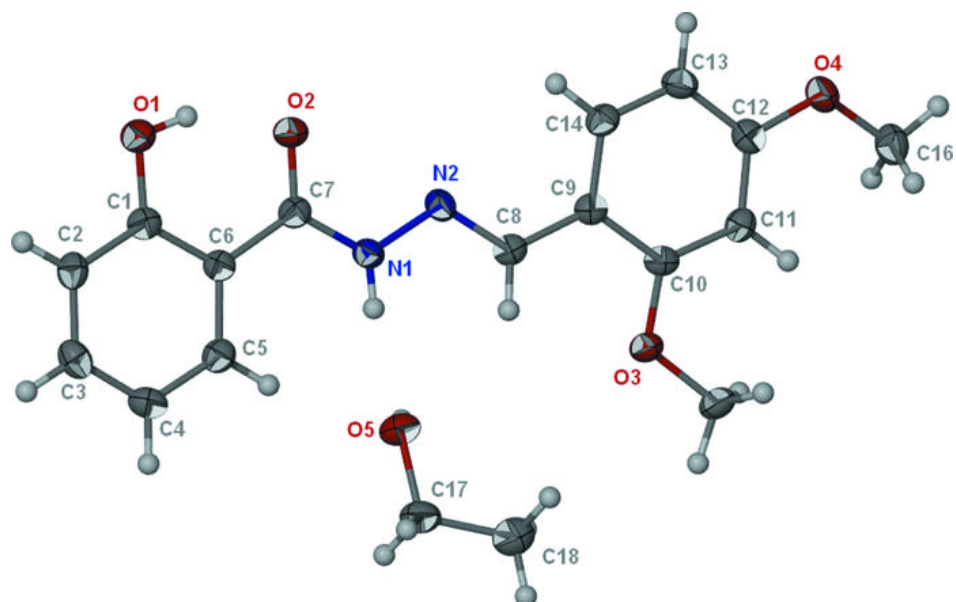


Fig. 2

