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(E)-N'-(3,4-Dimethoxybenzylidene)-2,4-dihydroxybenzohydrazide methanol solvate

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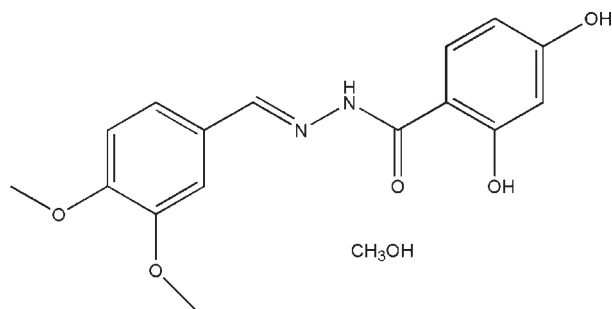
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.050; wR factor = 0.129; data-to-parameter ratio = 15.9.

The title compound, $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_5 \cdot \text{CH}_3\text{OH}$, was obtained from a condensation reaction of 3,4-dimethoxybenzaldehyde and 2,4-dihydroxybenzohydrazide. The non-H atoms of the Schiff base molecule are approximately coplanar (r.m.s. deviation = 0.043 Å) and the dihedral angle between the two benzene rings is 1.6 (1°). The molecule adopts an *E* configuration with respect to the $\text{C}=\text{N}$ double bond. An intramolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bond is observed. The Schiff base and methanol molecules are linked into a two-dimensional network parallel to $(10\bar{1})$ by intermolecular $\text{N}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds.

Related literature

For background to Schiff base compounds, hydrazone compounds and their biological properties, see: Kucukguzel *et al.* (2006); Khattab *et al.* (2005); Karthikeyan *et al.* (2006); Okabe *et al.* (1993). For bond-length data, see: Allen *et al.* (1987). For related structures, see: Shan *et al.* (2008); Fun *et al.* (2008); Ma *et al.* (2008); Diao *et al.* (2008a,b); Ejsmont *et al.* (2008).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_5 \cdot \text{CH}_4\text{O}$
 $M_r = 348.35$
 Monoclinic, $P2_1/n$
 $a = 8.497$ (1) Å
 $b = 17.431$ (2) Å
 $c = 11.933$ (2) Å
 $\beta = 102.93$ (2°)

$V = 1722.6$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 298$ K
 $0.25 \times 0.23 \times 0.23$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.975$, $T_{\max} = 0.977$

10465 measured reflections
 3732 independent reflections
 2017 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.129$
 $S = 1.03$
 3732 reflections
 235 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1A} \cdots \text{O2}^i$	0.90 (1)	2.217 (10)	3.108 (2)	170 (2)
$\text{O6}-\text{H6} \cdots \text{N2}^{ii}$	0.82	2.55	3.133 (2)	129
$\text{O6}-\text{H6} \cdots \text{O3}^{ii}$	0.82	2.02	2.807 (2)	161
$\text{O2}-\text{H2} \cdots \text{O6}^{iii}$	0.82	1.79	2.599 (2)	171
$\text{O1}-\text{H1} \cdots \text{O3}$	0.82	1.80	2.534 (2)	148

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$; (iii) $x + 1, y, z$.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2900).

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supplementary materials

Acta Cryst. (2009). E65, o2392-o2393 [doi:10.1107/S1600536809035752]

(*E*)-*N'*-(3,4-Dimethoxybenzylidene)-2,4-dihydroxybenzohydrazide methanol solvate

Q.-L. Zhang, L.-Z. Yin, X.-M. Deng, S.-C. Liu and D.-G. Song

Comment

Hydrazones and Schiff bases have been attracted much attention for their excellent biological properties, especially for their potential pharmacological and antitumor properties (Kucukguzel *et al.*, 2006; Khattab *et al.*, 2005; Karthikeyan *et al.*, 2006; Okabe *et al.*, 1993). Recently, a large number of hydrazone derivatives have been prepared and structurally characterized (Shan *et al.*, 2008; Fun *et al.*, 2008; Ma *et al.*, 2008; Diao *et al.*, 2008a,b; Ejsmont *et al.*, 2008). As part of the ongoing study, we report herein the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The compound consists of a Schiff base molecule and a methanol molecule. The dihedral angle between the two benzene rings is 1.6 (1)°. The Schiff base molecule displays an *E* configuration about the C=N bond. The bond lengths are typical (Allen *et al.*, 1987). The molecules are linked into a two-dimensional network parallel to the (10 $\bar{1}$) by intermolecular N—H \cdots O, O—H \cdots N, and O—H \cdots O hydrogen bonds (Fig. 2 and Table 1).

Experimental

3,4-Dimethoxybenzaldehyde (1.0 mmol, 166.2 mg) was dissolved in methanol (50 ml), then 2,4-dihydroxybenzohydrazide (1.0 mmol, 168.2 mg) was added slowly into the solution, and the mixture was kept at reflux with continuous stirring for 1 h. After the solution had cooled to room temperature colourless crystallites appeared. The crystallites were filtered and washed with methanol for three times. Recrystallization from an absolute methanol yielded block-shaped single crystals of the title compound.

Refinement

Atom H1A was located from a difference Fourier map and refined isotropically, with the N-H distance restrained to 0.90 (1) Å. Other H atoms were placed in calculated positions with C-H = 0.93-0.96 Å and O-H = 0.82 Å, and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{O and C}_{\text{methyl}})$. A rotating group model was used for methyl and hydroxyl groups.

Figures

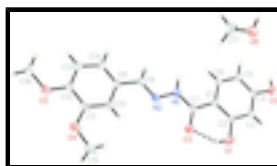


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates an intramolecular hydrogen bond.

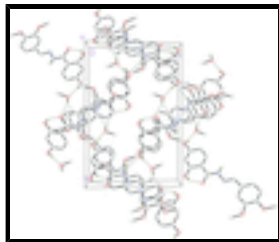


Fig. 2. The molecular packing of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

(*E*)-*N'*-(3,4-Dimethoxybenzylidene)-2,4-dihydroxybenzohydrazide methanol solvate

Crystal data

$C_{16}H_{16}N_2O_5 \cdot CH_4O$

$M_r = 348.35$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.497$ (1) Å

$b = 17.431$ (2) Å

$c = 11.933$ (2) Å

$\beta = 102.93$ (2)°

$V = 1722.6$ (4) Å³

$Z = 4$

$F_{000} = 736$

$D_x = 1.343$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1327 reflections

$\theta = 2.3$ – 24.5 °

$\mu = 0.10$ mm⁻¹

$T = 298$ K

Block, colourless

$0.25 \times 0.23 \times 0.23$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2001)

$T_{\min} = 0.975$, $T_{\max} = 0.977$

10465 measured reflections

3732 independent reflections

2017 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 27.0$ °

$\theta_{\min} = 2.1$ °

$h = -10 \rightarrow 10$

$k = -20 \rightarrow 22$

$l = -15 \rightarrow 7$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.129$

$S = 1.03$

3732 reflections

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

$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.0211P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.15$ e Å⁻³

235 parameters

$$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$$

1 restraint

Extinction correction: none

Primary atom site location: structure-invariant direct methods

Special details

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.9655 (2)	0.08862 (10)	0.61461 (15)	0.0408 (4)
N2	0.8536 (2)	0.03538 (10)	0.56016 (14)	0.0414 (4)
O1	1.2219 (2)	0.05972 (9)	0.95309 (12)	0.0623 (5)
H1	1.1561	0.0316	0.9118	0.093*
O2	1.52034 (18)	0.28449 (9)	0.94432 (11)	0.0499 (4)
H2	1.5442	0.3149	0.8984	0.075*
O3	1.01873 (19)	0.01674 (9)	0.77490 (12)	0.0544 (4)
O4	0.42243 (18)	-0.17176 (9)	0.40757 (13)	0.0562 (4)
O5	0.29676 (18)	-0.13286 (8)	0.19882 (13)	0.0582 (5)
O6	0.6296 (2)	0.37824 (9)	0.81028 (13)	0.0639 (5)
H6	0.5949	0.4222	0.8007	0.096*
C1	1.1618 (2)	0.13446 (11)	0.77945 (16)	0.0379 (5)
C2	1.2479 (3)	0.12222 (12)	0.89285 (17)	0.0419 (5)
C3	1.3640 (3)	0.17364 (13)	0.94638 (17)	0.0445 (5)
H3	1.4178	0.1655	1.0223	0.053*
C4	1.4008 (2)	0.23680 (12)	0.88820 (17)	0.0393 (5)
C5	1.3173 (3)	0.25089 (12)	0.77654 (17)	0.0461 (6)
H5	1.3401	0.2942	0.7375	0.055*
C6	1.2005 (2)	0.20011 (12)	0.72414 (17)	0.0442 (6)
H6A	1.1450	0.2098	0.6490	0.053*
C7	1.0444 (2)	0.07663 (12)	0.72359 (17)	0.0401 (5)
C8	0.7848 (2)	0.05124 (12)	0.45725 (18)	0.0412 (5)
H8	0.8152	0.0956	0.4242	0.049*
C9	0.6598 (2)	0.00287 (11)	0.38858 (17)	0.0373 (5)
C10	0.6063 (2)	-0.06345 (11)	0.43485 (17)	0.0408 (5)
H10	0.6532	-0.0781	0.5098	0.049*
C11	0.4845 (2)	-0.10693 (11)	0.36970 (18)	0.0414 (5)
C12	0.4150 (2)	-0.08531 (12)	0.25628 (18)	0.0434 (5)
C13	0.4679 (3)	-0.02028 (12)	0.21043 (18)	0.0479 (6)

supplementary materials

H13	0.4218	-0.0057	0.1353	0.057*
C14	0.5908 (3)	0.02357 (12)	0.27733 (17)	0.0443 (5)
H14	0.6267	0.0674	0.2463	0.053*
C15	0.4975 (3)	-0.19856 (14)	0.5184 (2)	0.0648 (7)
H15A	0.6088	-0.2100	0.5209	0.097*
H15B	0.4437	-0.2441	0.5353	0.097*
H15C	0.4912	-0.1597	0.5743	0.097*
C16	0.2220 (3)	-0.11211 (15)	0.0836 (2)	0.0661 (7)
H16A	0.1795	-0.0610	0.0826	0.099*
H16B	0.1358	-0.1473	0.0539	0.099*
H16C	0.3004	-0.1141	0.0369	0.099*
C17	0.6766 (4)	0.35311 (16)	0.7103 (2)	0.0814 (9)
H17A	0.7812	0.3736	0.7093	0.122*
H17B	0.5995	0.3705	0.6436	0.122*
H17C	0.6812	0.2981	0.7099	0.122*
H1A	0.979 (2)	0.1297 (8)	0.5719 (15)	0.050*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0420 (10)	0.0382 (11)	0.0393 (11)	-0.0067 (9)	0.0028 (8)	-0.0003 (8)
N2	0.0418 (10)	0.0372 (11)	0.0433 (11)	-0.0048 (8)	0.0056 (8)	-0.0044 (8)
O1	0.0787 (13)	0.0582 (11)	0.0429 (10)	-0.0152 (9)	-0.0014 (8)	0.0154 (8)
O2	0.0562 (10)	0.0511 (10)	0.0370 (9)	-0.0089 (8)	-0.0011 (7)	-0.0071 (7)
O3	0.0647 (11)	0.0474 (10)	0.0475 (10)	-0.0106 (8)	0.0049 (8)	0.0089 (7)
O4	0.0589 (10)	0.0405 (9)	0.0654 (11)	-0.0096 (8)	0.0057 (8)	0.0064 (8)
O5	0.0585 (10)	0.0475 (10)	0.0598 (11)	-0.0110 (8)	-0.0056 (8)	-0.0038 (8)
O6	0.0943 (14)	0.0413 (10)	0.0577 (11)	-0.0014 (10)	0.0201 (9)	-0.0022 (8)
C1	0.0427 (12)	0.0373 (12)	0.0311 (12)	0.0030 (10)	0.0031 (9)	0.0000 (9)
C2	0.0522 (13)	0.0417 (13)	0.0321 (12)	0.0043 (11)	0.0099 (10)	0.0038 (10)
C3	0.0528 (13)	0.0486 (14)	0.0286 (12)	0.0043 (11)	0.0012 (10)	-0.0003 (10)
C4	0.0408 (12)	0.0401 (13)	0.0340 (12)	0.0023 (10)	0.0023 (9)	-0.0099 (10)
C5	0.0559 (14)	0.0419 (14)	0.0354 (13)	-0.0025 (11)	-0.0005 (10)	0.0033 (10)
C6	0.0521 (13)	0.0445 (14)	0.0297 (12)	-0.0002 (11)	-0.0043 (10)	0.0016 (10)
C7	0.0419 (12)	0.0399 (13)	0.0367 (13)	0.0026 (10)	0.0048 (10)	0.0000 (10)
C8	0.0415 (12)	0.0352 (12)	0.0453 (14)	-0.0023 (10)	0.0063 (10)	-0.0015 (10)
C9	0.0368 (12)	0.0316 (12)	0.0419 (13)	-0.0005 (9)	0.0053 (9)	-0.0040 (9)
C10	0.0418 (12)	0.0368 (13)	0.0416 (13)	0.0029 (10)	0.0047 (10)	-0.0026 (10)
C11	0.0424 (12)	0.0294 (12)	0.0530 (14)	0.0006 (10)	0.0116 (10)	-0.0015 (10)
C12	0.0414 (12)	0.0339 (12)	0.0513 (15)	-0.0027 (10)	0.0026 (10)	-0.0103 (10)
C13	0.0506 (14)	0.0445 (14)	0.0446 (14)	-0.0028 (11)	0.0022 (11)	-0.0019 (11)
C14	0.0482 (13)	0.0377 (13)	0.0449 (14)	-0.0052 (10)	0.0059 (10)	0.0011 (10)
C15	0.0699 (17)	0.0456 (15)	0.0781 (19)	-0.0015 (13)	0.0147 (14)	0.0184 (13)
C16	0.0569 (15)	0.0674 (18)	0.0628 (18)	-0.0137 (14)	-0.0104 (12)	-0.0078 (13)
C17	0.114 (3)	0.072 (2)	0.0633 (19)	-0.0190 (18)	0.0304 (17)	-0.0166 (15)

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

N1—C7	1.339 (3)	C5—H5	0.93
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N1—N2	1.382 (2)	C6—H6A	0.93
N1—H1A	0.901 (9)	C8—C9	1.456 (3)
N2—C8	1.267 (2)	C8—H8	0.93
O1—C2	1.350 (2)	C9—C14	1.374 (3)
O1—H1	0.82	C9—C10	1.400 (3)
O2—C4	1.367 (2)	C10—C11	1.375 (3)
O2—H2	0.82	C10—H10	0.93
O3—C7	1.254 (2)	C11—C12	1.402 (3)
O4—C11	1.366 (2)	C12—C13	1.377 (3)
O4—C15	1.413 (3)	C13—C14	1.393 (3)
O5—C12	1.363 (2)	C13—H13	0.93
O5—C16	1.426 (3)	C14—H14	0.93
O6—C17	1.410 (3)	C15—H15A	0.96
O6—H6	0.82	C15—H15B	0.96
C1—C6	1.397 (3)	C15—H15C	0.96
C1—C2	1.403 (3)	C16—H16A	0.96
C1—C7	1.469 (3)	C16—H16B	0.96
C2—C3	1.380 (3)	C16—H16C	0.96
C3—C4	1.374 (3)	C17—H17A	0.96
C3—H3	0.93	C17—H17B	0.96
C4—C5	1.384 (3)	C17—H17C	0.96
C5—C6	1.372 (3)		
C7—N1—N2	119.58 (17)	C10—C9—C8	121.09 (19)
C7—N1—H1A	125.0 (14)	C11—C10—C9	120.1 (2)
N2—N1—H1A	115.4 (13)	C11—C10—H10	119.9
C8—N2—N1	115.41 (17)	C9—C10—H10	119.9
C2—O1—H1	109.5	O4—C11—C10	124.5 (2)
C4—O2—H2	109.5	O4—C11—C12	115.55 (18)
C11—O4—C15	117.13 (17)	C10—C11—C12	119.9 (2)
C12—O5—C16	116.74 (18)	O5—C12—C13	124.7 (2)
C17—O6—H6	109.5	O5—C12—C11	115.22 (19)
C6—C1—C2	116.94 (18)	C13—C12—C11	120.03 (19)
C6—C1—C7	123.76 (18)	C12—C13—C14	119.6 (2)
C2—C1—C7	119.21 (18)	C12—C13—H13	120.2
O1—C2—C3	117.58 (19)	C14—C13—H13	120.2
O1—C2—C1	121.59 (19)	C9—C14—C13	120.9 (2)
C3—C2—C1	120.83 (19)	C9—C14—H14	119.6
C4—C3—C2	120.42 (19)	C13—C14—H14	119.6
C4—C3—H3	119.8	O4—C15—H15A	109.5
C2—C3—H3	119.8	O4—C15—H15B	109.5
O2—C4—C3	117.89 (18)	H15A—C15—H15B	109.5
O2—C4—C5	121.9 (2)	O4—C15—H15C	109.5
C3—C4—C5	120.2 (2)	H15A—C15—H15C	109.5
C6—C5—C4	119.1 (2)	H15B—C15—H15C	109.5
C6—C5—H5	120.4	O5—C16—H16A	109.5
C4—C5—H5	120.4	O5—C16—H16B	109.5
C5—C6—C1	122.43 (19)	H16A—C16—H16B	109.5
C5—C6—H6A	118.8	O5—C16—H16C	109.5
C1—C6—H6A	118.8	H16A—C16—H16C	109.5

supplementary materials

O3—C7—N1	120.01 (19)	H16B—C16—H16C	109.5
O3—C7—C1	121.63 (19)	O6—C17—H17A	109.5
N1—C7—C1	118.35 (19)	O6—C17—H17B	109.5
N2—C8—C9	122.7 (2)	H17A—C17—H17B	109.5
N2—C8—H8	118.7	O6—C17—H17C	109.5
C9—C8—H8	118.7	H17A—C17—H17C	109.5
C14—C9—C10	119.45 (18)	H17B—C17—H17C	109.5
C14—C9—C8	119.44 (19)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O2 ⁱ	0.90 (1)	2.217 (10)	3.108 (2)	170 (2)
O6—H6 \cdots N2 ⁱⁱ	0.82	2.55	3.133 (2)	129
O6—H6 \cdots O3 ⁱⁱ	0.82	2.02	2.807 (2)	161
O2—H2 \cdots O6 ⁱⁱⁱ	0.82	1.79	2.599 (2)	171
O1—H1 \cdots O3	0.82	1.80	2.534 (2)	148

Symmetry codes: (i) $x-1/2, -y+1/2, z-1/2$; (ii) $-x+3/2, y+1/2, -z+3/2$; (iii) $x+1, y, z$.

Fig. 1

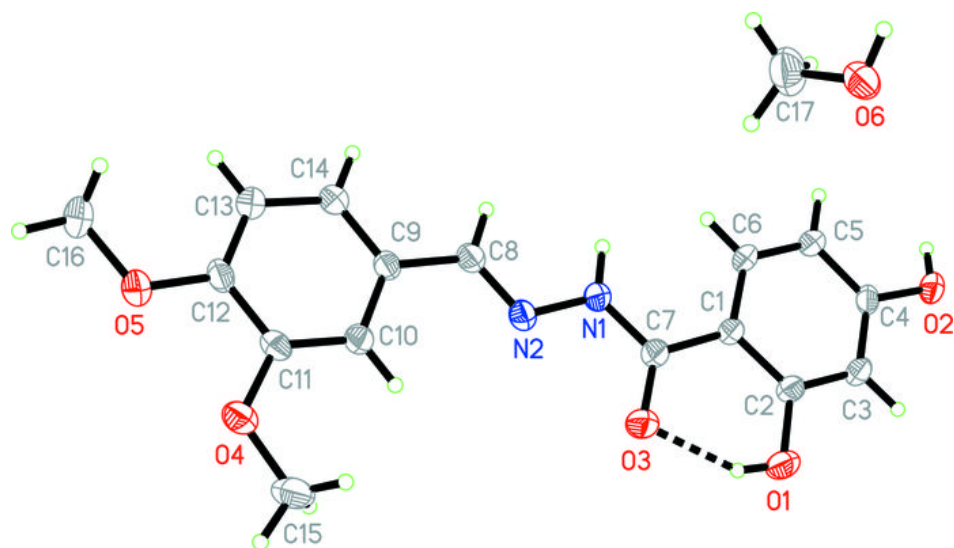


Fig. 2

