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(*E*)-4-Hydroxy-*N*′-(2-hydroxy-4-methoxybenzylidene)benzohydrazide *N*,*N*-dimethylformamide solvate

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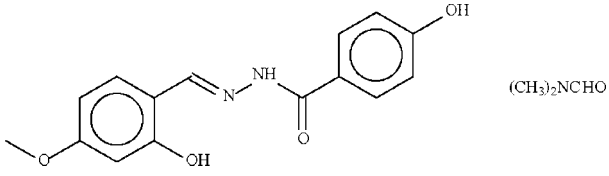
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 16.7.

The Schiff base molecule of the title compound, $C_{15}H_{14}N_2O_4\cdot C_3H_7NO$, adopts a *trans* configuration with respect to the C=N double bond; the Schiff base itself is nearly planar (r.m.s. deviation 0.20 Å). The amido N atom is a hydrogen-bond donor to the dimethylformamide solvate molecule. One of the hydroxy groups forms an intramolecular hydrogen bond to the N atom of the C=N double bond, whereas the other forms an intermolecular hydrogen bond to the carbonyl group.

Related literature

For the corresponding monohydrate, see: Lair *et al.* (2009).



Experimental

Crystal data

$C_{15}H_{14}N_2O_4\cdot C_3H_7NO$
M_r = 359.38
Monoclinic, $P2_1/c$
a = 11.8273 (2) Å
b = 7.8206 (2) Å
c = 19.4218 (3) Å
β = 103.674 (1)°
V = 1745.53 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 (2) K
0.30 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
11825 measured reflections
4003 independent reflections
3303 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.01
4003 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···O2^{i}	0.84	1.82	2.656 (1)	174
O3—H3o···N2	0.84	1.87	2.607 (1)	145
N1—H1n···O5	0.88	1.95	2.787 (1)	157

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

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, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2837).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
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Lair, N. M., Ali, H. M. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o189.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2009). E**65**, o190 [**doi:10.1107/S160053680804289X**]

(*E*)-4-Hydroxy-*N*'-(2-hydroxy-4-methoxybenzylidene)benzohydrazide *N*,*N*-dimethylformamide solvate

N. Mohd Lair, H. Mohd Ali and S. W. Ng

Comment

(type here to add)

Experimental

2-Hydroxy-3-methoxybenzaldehyde (0.30 g, 2 mmol) and 4-hydroxybenzohydrazide (0.30 g, 2 mmol) were heated in an ethanol-methanol mixture (50 ml) for 2 hours. The solvent was removed and the resulting compound recrystallized from DMF.

Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.95–0.98, N–H 0.88, O–H 0.84 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2–1.5 times U_{eq}(C,N,O).

Figures

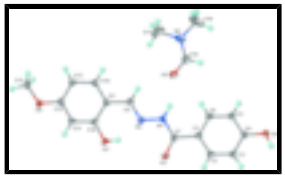

Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

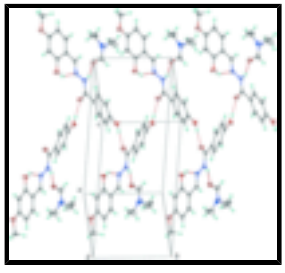

Fig. 2. Packing diagram with hydrogen bonds drawn as dashed lines.

(*E*)-4-Hydroxy-*N*'-(2-hydroxy-4-methoxybenzylidene)benzohydrazide *N*,*N*-dimethylformamide solvate

Crystal data

$C_{15}H_{14}N_2O_4{\cdot}C_3H_7NO$

M_r = 359.38

Monoclinic, $P2_1/c$

F_{000} = 760

D_x = 1.368 Mg m^{-3}

Mo $K\alpha$ radiation

λ = 0.71073 Å

Hall symbol: -P 2ybc	Cell parameters from 4180 reflections
a = 11.8273 (2) Å	θ = 2.2–28.3º
b = 7.8206 (2) Å	μ = 0.10 mm^{-1}
c = 19.4218 (3) Å	T = 100 (2) K
β = 103.674 (1)º	Prism, colorless
V = 1745.53 (6) Å^3	0.30 × 0.25 × 0.15 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	3303 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.023
Monochromator: graphite	θ_{max} = 27.5º
T = 100(2) K	θ_{min} = 2.2º
ω scans	h = −15→14
Absorption correction: None	k = −10→8
11825 measured reflections	l = −25→25
4003 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H-atom parameters constrained
$wR(F^2)$ = 0.104	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.678P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
4003 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
240 parameters	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.66809 (8)	0.74503 (12)	0.66928 (5)	0.0199 (2)
H1O	0.6979	0.7676	0.7120	0.030*
O2	0.22303 (8)	0.32357 (12)	0.69867 (4)	0.0211 (2)
O3	−0.04810 (8)	0.04690 (13)	0.62396 (5)	0.0228 (2)
H3O	0.0069	0.1161	0.6259	0.034*
O4	−0.40063 (8)	−0.13116 (12)	0.47806 (5)	0.0200 (2)
O5	0.18144 (8)	0.46309 (12)	0.44318 (5)	0.0227 (2)
N1	0.17427 (9)	0.37007 (14)	0.58062 (5)	0.0170 (2)
H1N	0.1888	0.4217	0.5434	0.020*
N2	0.07635 (9)	0.27015 (14)	0.57472 (5)	0.0173 (2)

N3	0.16184 (11)	0.57465 (17)	0.33359 (6)	0.0285 (3)
C1	0.35639 (10)	0.48355 (16)	0.64886 (6)	0.0154 (2)
C2	0.41943 (11)	0.53743 (17)	0.71534 (6)	0.0188 (3)
H2	0.3901	0.5146	0.7559	0.023*
C3	0.52370 (11)	0.62336 (17)	0.72326 (7)	0.0197 (3)
H3	0.5656	0.6584	0.7690	0.024*
C4	0.56747 (11)	0.65871 (16)	0.66420 (6)	0.0164 (3)
C5	0.50566 (11)	0.60607 (16)	0.59728 (6)	0.0179 (3)
H5	0.5351	0.6297	0.5568	0.022*
C6	0.40136 (11)	0.51936 (16)	0.58983 (6)	0.0174 (3)
H6	0.3597	0.4837	0.5441	0.021*
C7	0.24710 (11)	0.38628 (16)	0.64518 (6)	0.0162 (2)
C8	0.00648 (11)	0.25971 (16)	0.51315 (6)	0.0170 (3)
H8	0.0228	0.3201	0.4742	0.020*
C9	−0.09720 (10)	0.15539 (16)	0.50355 (6)	0.0158 (2)
C10	−0.12163 (11)	0.05447 (16)	0.55883 (6)	0.0169 (3)
C11	−0.22325 (11)	−0.04046 (16)	0.54772 (6)	0.0178 (3)
H11	−0.2388	−0.1090	0.5848	0.021*
C12	−0.30237 (11)	−0.03528 (16)	0.48223 (7)	0.0169 (3)
C13	−0.28026 (11)	0.06116 (16)	0.42650 (7)	0.0183 (3)
H13	−0.3341	0.0633	0.3817	0.022*
C14	−0.17781 (11)	0.15370 (16)	0.43817 (6)	0.0173 (3)
H14	−0.1617	0.2186	0.4002	0.021*
C15	−0.49470 (11)	−0.10776 (18)	0.41743 (7)	0.0208 (3)
H15A	−0.5643	−0.1651	0.4252	0.031*
H15B	−0.4739	−0.1568	0.3757	0.031*
H15C	−0.5105	0.0147	0.4098	0.031*
C16	0.21144 (11)	0.56143 (17)	0.40187 (7)	0.0217 (3)
H16	0.2757	0.6343	0.4204	0.026*
C17	0.06495 (16)	0.4656 (3)	0.30112 (9)	0.0449 (5)
H17A	0.0502	0.3839	0.3362	0.067*
H17B	0.0836	0.4033	0.2614	0.067*
H17C	−0.0045	0.5358	0.2837	0.067*
C18	0.20628 (17)	0.6926 (3)	0.28847 (10)	0.0555 (6)
H18A	0.2725	0.7558	0.3170	0.083*
H18B	0.1448	0.7731	0.2665	0.083*
H18C	0.2315	0.6283	0.2514	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0186 (4)	0.0259 (5)	0.0151 (4)	−0.0060 (4)	0.0037 (3)	−0.0012 (4)
O2	0.0185 (4)	0.0274 (5)	0.0168 (4)	−0.0028 (4)	0.0030 (3)	0.0036 (4)
O3	0.0202 (5)	0.0306 (6)	0.0156 (4)	−0.0057 (4)	0.0005 (4)	0.0032 (4)
O4	0.0167 (4)	0.0236 (5)	0.0188 (4)	−0.0051 (4)	0.0026 (4)	0.0005 (4)
O5	0.0268 (5)	0.0235 (5)	0.0173 (4)	−0.0020 (4)	0.0044 (4)	0.0008 (4)
N1	0.0158 (5)	0.0190 (5)	0.0155 (5)	−0.0034 (4)	0.0023 (4)	0.0013 (4)
N2	0.0149 (5)	0.0180 (5)	0.0191 (5)	−0.0012 (4)	0.0040 (4)	−0.0011 (4)

N3	0.0272 (6)	0.0369 (7)	0.0224 (6)	0.0071 (5)	0.0079 (5)	0.0088 (5)
C1	0.0155 (6)	0.0138 (6)	0.0166 (6)	0.0017 (5)	0.0027 (5)	0.0003 (4)
C2	0.0213 (6)	0.0210 (7)	0.0146 (6)	−0.0028 (5)	0.0054 (5)	−0.0002 (5)
C3	0.0224 (6)	0.0220 (7)	0.0140 (6)	−0.0037 (5)	0.0031 (5)	−0.0019 (5)
C4	0.0156 (6)	0.0152 (6)	0.0180 (6)	0.0003 (5)	0.0033 (5)	0.0004 (5)
C5	0.0196 (6)	0.0196 (6)	0.0155 (6)	0.0004 (5)	0.0058 (5)	0.0003 (5)
C6	0.0183 (6)	0.0188 (6)	0.0138 (6)	0.0009 (5)	0.0013 (5)	−0.0008 (5)
C7	0.0157 (6)	0.0159 (6)	0.0168 (6)	0.0021 (5)	0.0032 (5)	−0.0002 (5)
C8	0.0178 (6)	0.0168 (6)	0.0168 (6)	0.0008 (5)	0.0050 (5)	0.0004 (5)
C9	0.0146 (6)	0.0156 (6)	0.0173 (6)	0.0011 (5)	0.0041 (5)	−0.0013 (5)
C10	0.0167 (6)	0.0190 (6)	0.0145 (6)	0.0024 (5)	0.0028 (5)	−0.0008 (5)
C11	0.0195 (6)	0.0189 (6)	0.0161 (6)	0.0009 (5)	0.0064 (5)	0.0018 (5)
C12	0.0151 (6)	0.0160 (6)	0.0203 (6)	−0.0003 (5)	0.0055 (5)	−0.0027 (5)
C13	0.0173 (6)	0.0210 (7)	0.0156 (6)	0.0012 (5)	0.0016 (5)	−0.0002 (5)
C14	0.0189 (6)	0.0179 (6)	0.0151 (6)	0.0012 (5)	0.0042 (5)	0.0022 (5)
C15	0.0163 (6)	0.0252 (7)	0.0198 (6)	−0.0030 (5)	0.0022 (5)	−0.0017 (5)
C16	0.0197 (6)	0.0211 (7)	0.0239 (6)	0.0011 (5)	0.0045 (5)	0.0008 (5)
C17	0.0402 (10)	0.0651 (13)	0.0238 (8)	0.0006 (9)	−0.0040 (7)	−0.0066 (8)
C18	0.0496 (11)	0.0763 (15)	0.0460 (11)	0.0161 (10)	0.0217 (9)	0.0405 (10)

Geometric parameters (Å, °)

O1—C4	1.3514 (15)	C5—H5	0.9500
O1—H1O	0.8400	C6—H6	0.9500
O2—C7	1.2412 (15)	C8—C9	1.4478 (17)
O3—C10	1.3565 (15)	C8—H8	0.9500
O3—H3O	0.8400	C9—C14	1.3962 (17)
O4—C12	1.3693 (15)	C9—C10	1.4162 (17)
O4—C15	1.4278 (15)	C10—C11	1.3855 (17)
O5—C16	1.2229 (16)	C11—C12	1.3901 (17)
N1—C7	1.3489 (15)	C11—H11	0.9500
N1—N2	1.3791 (14)	C12—C13	1.3938 (17)
N1—H1N	0.8800	C13—C14	1.3832 (17)
N2—C8	1.2855 (16)	C13—H13	0.9500
N3—C16	1.3212 (17)	C14—H14	0.9500
N3—C17	1.448 (2)	C15—H15A	0.9800
N3—C18	1.454 (2)	C15—H15B	0.9800
C1—C2	1.3948 (17)	C15—H15C	0.9800
C1—C6	1.4013 (17)	C16—H16	0.9500
C1—C7	1.4870 (17)	C17—H17A	0.9800
C2—C3	1.3808 (18)	C17—H17B	0.9800
C2—H2	0.9500	C17—H17C	0.9800
C3—C4	1.3931 (17)	C18—H18A	0.9800
C3—H3	0.9500	C18—H18B	0.9800
C4—C5	1.3943 (17)	C18—H18C	0.9800
C5—C6	1.3850 (17)		
C4—O1—H1O	109.5	O3—C10—C11	117.60 (11)
C10—O3—H3O	109.5	O3—C10—C9	122.04 (11)
C12—O4—C15	117.61 (10)	C11—C10—C9	120.36 (11)

C7—N1—N2	118.01 (10)	C10—C11—C12	119.89 (11)
C7—N1—H1N	121.0	C10—C11—H11	120.1
N2—N1—H1N	121.0	C12—C11—H11	120.1
C8—N2—N1	117.12 (10)	O4—C12—C11	114.61 (11)
C16—N3—C17	120.60 (13)	O4—C12—C13	124.26 (11)
C16—N3—C18	121.12 (14)	C11—C12—C13	121.13 (11)
C17—N3—C18	118.21 (14)	C14—C13—C12	118.28 (11)
C2—C1—C6	118.28 (11)	C14—C13—H13	120.9
C2—C1—C7	117.86 (11)	C12—C13—H13	120.9
C6—C1—C7	123.83 (11)	C13—C14—C9	122.50 (11)
C3—C2—C1	121.20 (11)	C13—C14—H14	118.7
C3—C2—H2	119.4	C9—C14—H14	118.7
C1—C2—H2	119.4	O4—C15—H15A	109.5
C2—C3—C4	120.06 (12)	O4—C15—H15B	109.5
C2—C3—H3	120.0	H15A—C15—H15B	109.5
C4—C3—H3	120.0	O4—C15—H15C	109.5
O1—C4—C3	122.10 (11)	H15A—C15—H15C	109.5
O1—C4—C5	118.30 (11)	H15B—C15—H15C	109.5
C3—C4—C5	119.60 (11)	O5—C16—N3	125.37 (13)
C6—C5—C4	119.98 (11)	O5—C16—H16	117.3
C6—C5—H5	120.0	N3—C16—H16	117.3
C4—C5—H5	120.0	N3—C17—H17A	109.5
C5—C6—C1	120.89 (11)	N3—C17—H17B	109.5
C5—C6—H6	119.6	H17A—C17—H17B	109.5
C1—C6—H6	119.6	N3—C17—H17C	109.5
O2—C7—N1	121.23 (11)	H17A—C17—H17C	109.5
O2—C7—C1	122.05 (11)	H17B—C17—H17C	109.5
N1—C7—C1	116.72 (11)	N3—C18—H18A	109.5
N2—C8—C9	119.62 (11)	N3—C18—H18B	109.5
N2—C8—H8	120.2	H18A—C18—H18B	109.5
C9—C8—H8	120.2	N3—C18—H18C	109.5
C14—C9—C10	117.80 (11)	H18A—C18—H18C	109.5
C14—C9—C8	119.86 (11)	H18B—C18—H18C	109.5
C10—C9—C8	122.34 (11)		
C7—N1—N2—C8	178.29 (11)	N2—C8—C9—C10	−4.09 (18)
C6—C1—C2—C3	−0.22 (19)	C14—C9—C10—O3	179.47 (11)
C7—C1—C2—C3	177.82 (12)	C8—C9—C10—O3	−1.25 (19)
C1—C2—C3—C4	0.4 (2)	C14—C9—C10—C11	−0.74 (18)
C2—C3—C4—O1	178.84 (12)	C8—C9—C10—C11	178.55 (11)
C2—C3—C4—C5	−0.3 (2)	O3—C10—C11—C12	179.08 (11)
O1—C4—C5—C6	−179.11 (11)	C9—C10—C11—C12	−0.72 (19)
C3—C4—C5—C6	0.07 (19)	C15—O4—C12—C11	168.75 (11)
C4—C5—C6—C1	0.10 (19)	C15—O4—C12—C13	−11.33 (17)
C2—C1—C6—C5	−0.02 (19)	C10—C11—C12—O4	−178.59 (11)
C7—C1—C6—C5	−177.94 (12)	C10—C11—C12—C13	1.49 (19)
N2—N1—C7—O2	−5.05 (18)	O4—C12—C13—C14	179.34 (11)
N2—N1—C7—C1	175.38 (10)	C11—C12—C13—C14	−0.74 (19)
C2—C1—C7—O2	−14.53 (18)	C12—C13—C14—C9	−0.79 (19)
C6—C1—C7—O2	163.40 (12)	C10—C9—C14—C13	1.52 (18)

C2—C1—C7—N1	165.03 (11)	C8—C9—C14—C13	−177.79 (12)
C6—C1—C7—N1	−17.04 (18)	C17—N3—C16—O5	−1.2 (2)
N1—N2—C8—C9	179.42 (11)	C18—N3—C16—O5	−178.22 (15)
N2—C8—C9—C14	175.18 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···O2^{i}	0.84	1.82	2.656 (1)	174
O3—H3o···N2	0.84	1.87	2.607 (1)	145
N1—H1n···O5	0.88	1.95	2.787 (1)	157

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1

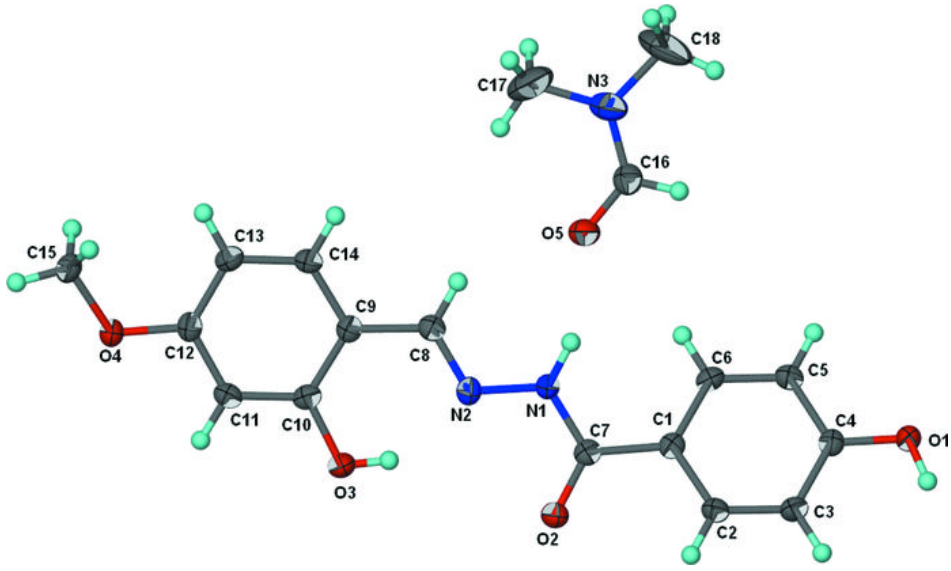
C18
C17
N3
C16
O5
C15
C13
C14
C9
O4
C12
C8
C6
C5
C11
C10
N2
N1
C7
C1
C4
O1
O3
O2
C2
C3

Fig. 2