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(*E*)-3-(2-Hydroxy-5-methylphenylimino)-indolin-2-one

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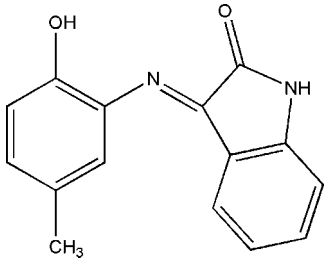
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.114; data-to-parameter ratio = 12.6.

In the title compound, $C_{15}H_{12}N_2O_2$, the dihedral angle between the two benzene rings is 83.55 (11)° In the crystal, the molecules are linked by O—H···O and N—H···O hydrogen bonds.

Related literature

For general background on Schiff base ligands, see: Guo *et al.* (2011); Drozdzak *et al.* (2005); Weber *et al.* (2007); Liu *et al.* (2010). For standard bond lengths, see: Allen *et al.* (1987)



Experimental

Crystal data

$C_{15}H_{12}N_2O_2$
M_r = 252.27
Monoclinic, $P2_1/c$
a = 12.6211 (11) Å
b = 8.7100 (7) Å
c = 11.2835 (10) Å
β = 90.780 (1)°
V = 1240.28 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.50 × 0.47 × 0.17 mm

Data collection

CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.956, T_{max} = 0.985
5982 measured reflections
2182 independent reflections
1449 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.114
S = 1.02
2182 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.86	2.6729 (19)	169
N1—H1···O2^{ii}	0.86	2.06	2.842 (2)	151

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2008).

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supporting information

Acta Cryst. (2011). E**67**, o2493 [doi:10.1107/S1600536811034015]

(*E*)-3-(2-Hydroxy-5-methylphenylimino)indolin-2-one

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S1. Comment

Being one of the most prevalent sustems in coordination chemistry, Schiff base ligands have received much attention in recent years (Guo *et al.*, 2011), primarily due to their importance in metal complexes with catalytic activities (Drozdzak *et al.*, 2005), special magnetism (Weber *et al.*, 2007) and biological properties, for example, anticancer activities (Liu *et al.*, 2010). In the present paper, the synthesis and structure of a new Schiff base ligand is reported.

The crystal structure of the new ligand is given in Fig.1. The molecular structure of the compound is not coplanar, the dihedral angle between the two benzene rings is 83.55 °, it is almost perpendicular. The bond lengths and angles (Table 1) are within normal values (Allen *et al.*,1987). In the crystal structure, the adjacent molecules are linked through 0—H···0 and N—H···O hydrogen bonding (Table 2), to generate one-dimensional chain in direction (Fig.2).

S2. Experimental

2,3-indolinedione (5 mmol, 0.736 g) was dissolved in anhydrous ethanol (20 ml), then an anhydrous ethanol solution (10 ml) of 2-amino-4-methylphenol (5 mmol, 0.612 g) was slowly added. The mixture was refluxed for 4 h at 333k,and then cooled down to room temperature. A dark brown solid separated out. The solid was filtered off, washed several times with anhydrous ethanol and dried in vacuum drier. The dark brown single-crystal of the title ligand suitable for X-ray diffraction was trained in anhydrous ethanol at room temperature.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C—H = 0.96 Å (methyl), 0.93 Å (methenyl), 0.93 Å (aromatic), and U_{iso}(H) =1.2U_{eq}(C).

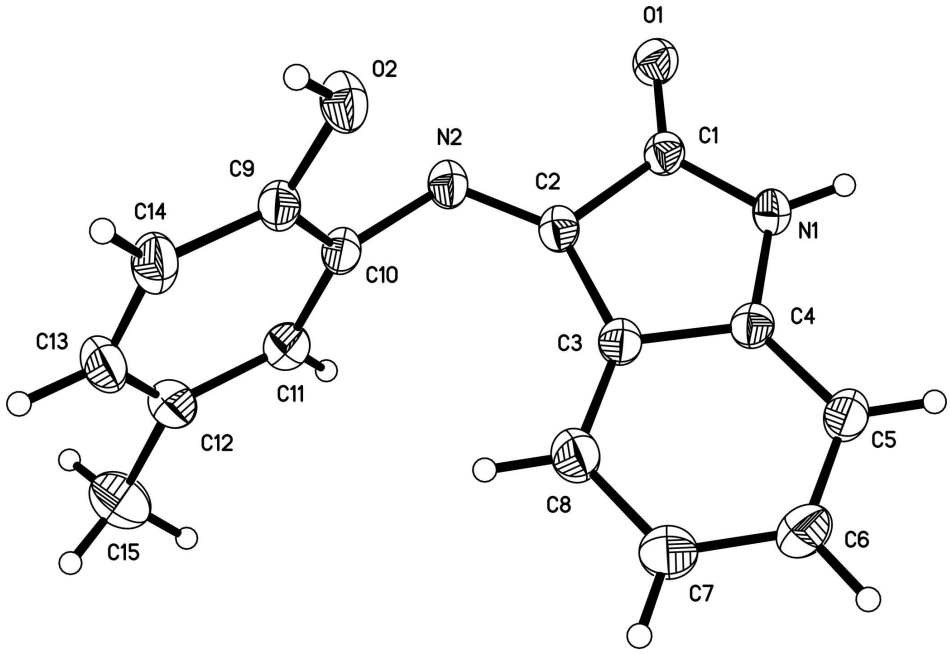

Figure 1

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

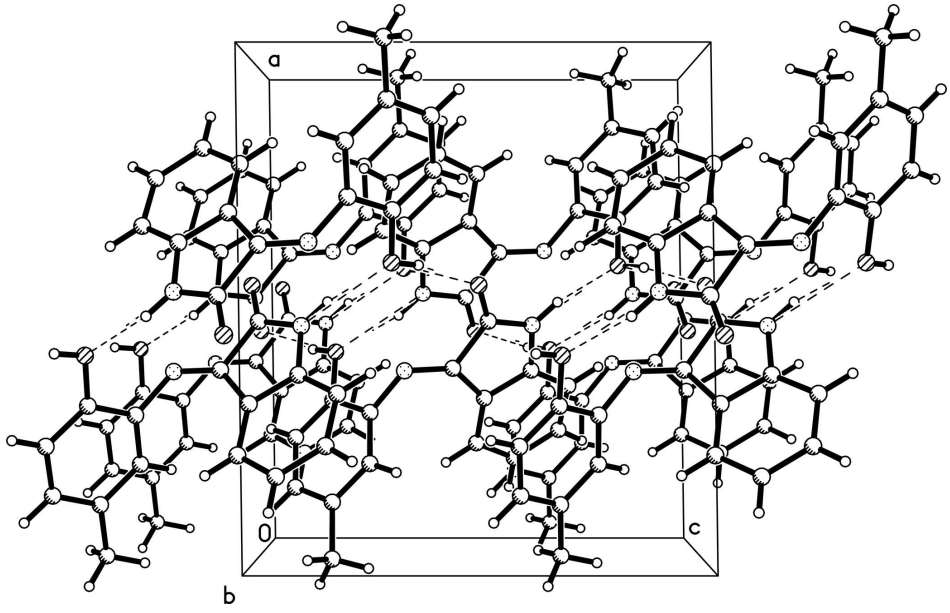

Figure 2

A view of the crystal structure showing chain to the *c* linked *via* O—H···O and N—H···O contacts.

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c = 11.2835 (10) Å
β = 90.780 (1)°

V = 1240.28 (18) Å^3
Z = 4
F(000) = 528
D_x = 1.351 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1807 reflections

θ = 2.8–25.8°
μ = 0.09 mm^{-1}
T = 298 K
Block, dark-brown
0.50 × 0.47 × 0.17 mm

Data collection

CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.956, T_{max} = 0.985

5982 measured reflections
2182 independent reflections
1449 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 25.0°, θ_{min} = 2.8°
h = −14→14
k = −10→10
l = −10→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.114
S = 1.02
2182 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.3363P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.017 (2)

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
N1	0.53216 (12)	0.37862 (19)	0.37637 (13)	0.0391 (4)
H1	0.4865	0.3785	0.3191	0.047*
N2	0.62133 (12)	0.28888 (19)	0.66041 (14)	0.0404 (4)
O1	0.45391 (11)	0.19850 (16)	0.49452 (12)	0.0474 (4)
O2	0.58728 (11)	0.51425 (16)	0.82237 (12)	0.0490 (4)
H2	0.5830	0.5750	0.8776	0.073*
C1	0.52386 (15)	0.2918 (2)	0.47439 (16)	0.0358 (5)
C2	0.61738 (14)	0.3381 (2)	0.55449 (16)	0.0355 (5)
C3	0.67930 (15)	0.4476 (2)	0.48520 (17)	0.0384 (5)

C4	0.62382 (14)	0.4693 (2)	0.37841 (17)	0.0369 (5)
C5	0.65726 (16)	0.5680 (2)	0.29187 (18)	0.0465 (5)
H5	0.6188	0.5816	0.2218	0.056*
C6	0.75054 (18)	0.6460 (3)	0.3136 (2)	0.0564 (6)
H6	0.7756	0.7137	0.2567	0.068*
C7	0.80770 (18)	0.6262 (3)	0.4179 (2)	0.0611 (7)
H7	0.8704	0.6805	0.4299	0.073*
C8	0.77297 (16)	0.5266 (3)	0.5045 (2)	0.0519 (6)
H8	0.8118	0.5131	0.5744	0.062*
C9	0.68333 (15)	0.4423 (2)	0.82729 (17)	0.0400 (5)
C10	0.70454 (15)	0.3352 (2)	0.73941 (16)	0.0398 (5)
C11	0.80213 (16)	0.2627 (3)	0.73843 (19)	0.0496 (6)
H11	0.8161	0.1920	0.6789	0.059*
C12	0.87940 (17)	0.2925 (3)	0.8235 (2)	0.0566 (6)
C13	0.85588 (18)	0.3980 (3)	0.9110 (2)	0.0596 (7)
H13	0.9064	0.4195	0.9695	0.072*
C14	0.75915 (17)	0.4720 (3)	0.91347 (19)	0.0516 (6)
H14	0.7451	0.5421	0.9734	0.062*
C15	0.98450 (19)	0.2096 (4)	0.8213 (3)	0.0907 (10)
H15A	1.0391	0.2757	0.8522	0.136*
H15B	1.0006	0.1817	0.7412	0.136*
H15C	0.9806	0.1186	0.8691	0.136*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0391 (9)	0.0482 (10)	0.0300 (9)	0.0008 (8)	−0.0053 (7)	0.0017 (8)
N2	0.0432 (9)	0.0452 (10)	0.0326 (9)	0.0010 (8)	−0.0054 (7)	−0.0002 (8)
O1	0.0487 (8)	0.0530 (9)	0.0403 (8)	−0.0093 (7)	−0.0018 (6)	0.0006 (7)
O2	0.0542 (9)	0.0530 (9)	0.0395 (8)	0.0082 (7)	−0.0098 (7)	−0.0066 (7)
C1	0.0389 (11)	0.0384 (12)	0.0300 (11)	0.0044 (9)	0.0008 (8)	−0.0030 (9)
C2	0.0397 (10)	0.0358 (11)	0.0311 (11)	0.0069 (9)	−0.0014 (8)	−0.0030 (9)
C3	0.0399 (11)	0.0400 (12)	0.0352 (11)	0.0019 (9)	−0.0009 (9)	0.0006 (9)
C4	0.0391 (11)	0.0383 (12)	0.0335 (11)	0.0057 (9)	0.0028 (8)	−0.0010 (9)
C5	0.0520 (13)	0.0494 (13)	0.0380 (12)	0.0034 (11)	0.0011 (10)	0.0066 (10)
C6	0.0611 (14)	0.0521 (15)	0.0562 (15)	−0.0070 (12)	0.0071 (12)	0.0141 (12)
C7	0.0560 (14)	0.0610 (16)	0.0660 (16)	−0.0177 (12)	−0.0049 (12)	0.0104 (13)
C8	0.0507 (13)	0.0544 (15)	0.0502 (13)	−0.0066 (11)	−0.0090 (10)	0.0062 (11)
C9	0.0425 (12)	0.0432 (12)	0.0341 (11)	−0.0041 (9)	−0.0055 (9)	0.0061 (10)
C10	0.0424 (11)	0.0466 (13)	0.0302 (11)	−0.0049 (10)	−0.0037 (8)	0.0053 (9)
C11	0.0457 (12)	0.0609 (15)	0.0421 (13)	0.0020 (11)	0.0026 (10)	0.0035 (11)
C12	0.0414 (12)	0.0746 (17)	0.0537 (14)	−0.0034 (12)	−0.0054 (10)	0.0126 (13)
C13	0.0507 (14)	0.0753 (18)	0.0523 (15)	−0.0169 (13)	−0.0190 (11)	0.0100 (14)
C14	0.0597 (14)	0.0541 (14)	0.0405 (13)	−0.0083 (12)	−0.0115 (10)	0.0005 (11)
C15	0.0469 (14)	0.133 (3)	0.092 (2)	0.0122 (17)	−0.0062 (14)	0.013 (2)

Geometric parameters (Å, º)

N1—C1	1.345 (2)	C7—C8	1.383 (3)
N1—C4	1.401 (2)	C7—H7	0.9300
N1—H1	0.8600	C8—H8	0.9300
N2—C2	1.270 (2)	C9—C14	1.380 (3)
N2—C10	1.427 (2)	C9—C10	1.390 (3)
O1—C1	1.223 (2)	C10—C11	1.384 (3)
O2—C9	1.365 (2)	C11—C12	1.383 (3)
O2—H2	0.8200	C11—H11	0.9300
C1—C2	1.531 (3)	C12—C13	1.384 (3)
C2—C3	1.466 (3)	C12—C15	1.511 (3)
C3—C8	1.383 (3)	C13—C14	1.381 (3)
C3—C4	1.398 (3)	C13—H13	0.9300
C4—C5	1.372 (3)	C14—H14	0.9300
C5—C6	1.379 (3)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C6—C7	1.383 (3)	C15—H15C	0.9600
C6—H6	0.9300		
C1—N1—C4	112.15 (16)	C3—C8—H8	120.7
C1—N1—H1	123.9	C7—C8—H8	120.7
C4—N1—H1	123.9	O2—C9—C14	123.33 (19)
C2—N2—C10	120.77 (17)	O2—C9—C10	117.30 (17)
C9—O2—H2	109.5	C14—C9—C10	119.36 (19)
O1—C1—N1	126.19 (18)	C11—C10—C9	119.46 (18)
O1—C1—C2	128.17 (17)	C11—C10—N2	120.89 (19)
N1—C1—C2	105.61 (16)	C9—C10—N2	119.23 (17)
N2—C2—C3	135.01 (18)	C12—C11—C10	121.9 (2)
N2—C2—C1	119.12 (17)	C12—C11—H11	119.1
C3—C2—C1	105.61 (15)	C10—C11—H11	119.1
C8—C3—C4	119.07 (19)	C11—C12—C13	117.6 (2)
C8—C3—C2	134.48 (18)	C11—C12—C15	120.7 (2)
C4—C3—C2	106.45 (16)	C13—C12—C15	121.7 (2)
C5—C4—C3	122.87 (19)	C14—C13—C12	121.5 (2)
C5—C4—N1	127.13 (18)	C14—C13—H13	119.2
C3—C4—N1	109.99 (17)	C12—C13—H13	119.2
C4—C5—C6	116.9 (2)	C9—C14—C13	120.2 (2)
C4—C5—H5	121.5	C9—C14—H14	119.9
C6—C5—H5	121.5	C13—C14—H14	119.9
C5—C6—C7	121.6 (2)	C12—C15—H15A	109.5
C5—C6—H6	119.2	C12—C15—H15B	109.5
C7—C6—H6	119.2	H15A—C15—H15B	109.5
C6—C7—C8	120.9 (2)	C12—C15—H15C	109.5
C6—C7—H7	119.6	H15A—C15—H15C	109.5
C8—C7—H7	119.6	H15B—C15—H15C	109.5
C3—C8—C7	118.6 (2)		

C4—N1—C1—O1	−177.50 (18)	C4—C5—C6—C7	−0.2 (3)
C4—N1—C1—C2	4.1 (2)	C5—C6—C7—C8	0.0 (4)
C10—N2—C2—C3	−4.0 (3)	C4—C3—C8—C7	0.9 (3)
C10—N2—C2—C1	−177.06 (16)	C2—C3—C8—C7	−178.5 (2)
O1—C1—C2—N2	−7.8 (3)	C6—C7—C8—C3	−0.4 (4)
N1—C1—C2—N2	170.58 (17)	O2—C9—C10—C11	177.98 (17)
O1—C1—C2—C3	177.25 (18)	C14—C9—C10—C11	−1.3 (3)
N1—C1—C2—C3	−4.36 (19)	O2—C9—C10—N2	−9.3 (3)
N2—C2—C3—C8	8.8 (4)	C14—C9—C10—N2	171.34 (18)
C1—C2—C3—C8	−177.5 (2)	C2—N2—C10—C11	−82.8 (2)
N2—C2—C3—C4	−170.7 (2)	C2—N2—C10—C9	104.6 (2)
C1—C2—C3—C4	3.1 (2)	C9—C10—C11—C12	0.7 (3)
C8—C3—C4—C5	−1.1 (3)	N2—C10—C11—C12	−171.90 (19)
C2—C3—C4—C5	178.45 (18)	C10—C11—C12—C13	0.2 (3)
C8—C3—C4—N1	179.66 (17)	C10—C11—C12—C15	179.0 (2)
C2—C3—C4—N1	−0.8 (2)	C11—C12—C13—C14	−0.4 (3)
C1—N1—C4—C5	178.56 (19)	C15—C12—C13—C14	−179.1 (2)
C1—N1—C4—C3	−2.2 (2)	O2—C9—C14—C13	−178.12 (19)
C3—C4—C5—C6	0.7 (3)	C10—C9—C14—C13	1.2 (3)
N1—C4—C5—C6	179.83 (19)	C12—C13—C14—C9	−0.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.86	2.6729 (19)	169
N1—H1···O2^{ii}	0.86	2.06	2.842 (2)	151

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