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2-Methyl-1*H*-indole-3-carbaldehyde 4-hydroxybenzoylhydrazone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.124
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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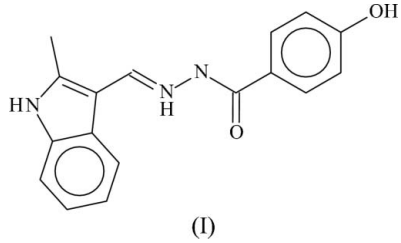
The NH group of the methylindolecarbaldehyde moiety and the OH group of the hydroxybenzoylhydrazone moiety of the title compound, $C_{17}H_{15}N_3O_2$, interact to form a linear chain; adjacent chains are linked through the amide –N(H)—C(═O)– portion of the molecule to form a tightly held three-dimensional network structure.

Comment

This study continues our work on Schiff bases that are formed by condensing 2-methylindole-3-carbaldehyde with an aroylhydrazine (Ali *et al.*, 2006). In the title molecule, (I) (Fig. 1), the amine group of the methylindole-3-carbaldehyde moiety interacts with the hydroxy group of the hydroxybenzoylhydrazine moiety of a neighboring molecule to form a linear chain. In the –N(H)–C(═O)– portion, the –NH unit serves as a hydrogen-bond donor and the C═O unit as a hydrogen-bond acceptor (Table 1), these hydrogen-bonding interactions consolidating the three-dimensional network into a tightly held architecture.



(I)

Experimental

2-Methylindole-3-carbaldehyde (0.44, 2.7 mmol) and 4-hydroxybenzhydrazide (0.42 g, 2.7 mmol) were heated in ethanol (100 ml) for 2 h. The solvent was removed and the pure compound obtained by recrystallization from dimethylformamide.

Crystal data

$C_{17}H_{15}N_3O_2$
M_r = 293.32
Monoclinic, $P2_1/c$
a = 12.171 (1) Å
b = 14.090 (1) Å
c = 8.6767 (7) Å
β = 97.917 (1)°
V = 1473.8 (2) Å^3
Z = 4
D_x = 1.322 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
Block, yellow
0.31 × 0.27 × 0.24 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: none
13436 measured reflections
3236 independent reflections
2516 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.124$
$S = 1.04$
3236 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.3578P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2o···O1^{i}	0.85 (1)	1.85 (1)	2.700 (2)	175 (2)
N1—H1n···O2^{ii}	0.86 (1)	2.07 (1)	2.910 (2)	164 (2)
N3—H3n···O1^{iii}	0.86 (1)	2.07 (1)	2.933 (2)	174 (2)

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

C-bound H atoms were placed at calculated positions (C—H = 0.93–0.96 Å) and included in the refinement in the riding-model approximation, with U_{iso}(H) values set at 1.2–1.5U_{eq}(C). The N- and O-bound H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = N—H = 0.85 (1) Å; their displacement parameters were freely refined.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

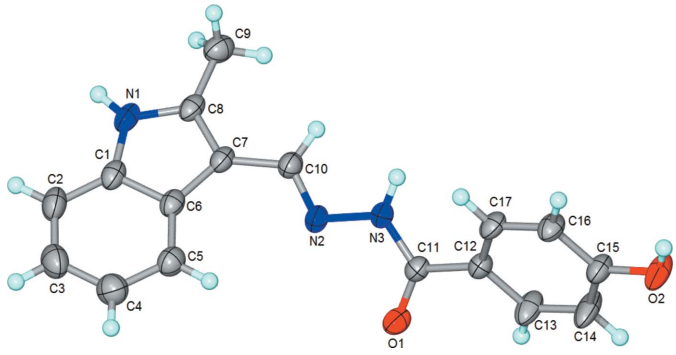


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level and H atoms as spheres of arbitrary radii.

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