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5-Chloro-1*H*-indole-3-carbaldehyde benzoylhydrazone

Hapipah M. Ali,[a] Mohd Idris Najwa,[a] Ming-Jin Xie[b] and Seik Weng Ng[a]*

[a]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [b]School Chemistry, Yunnan University, Kunming 650092, People's Republic of China

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.106
Data-to-parameter ratio = 15.8

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

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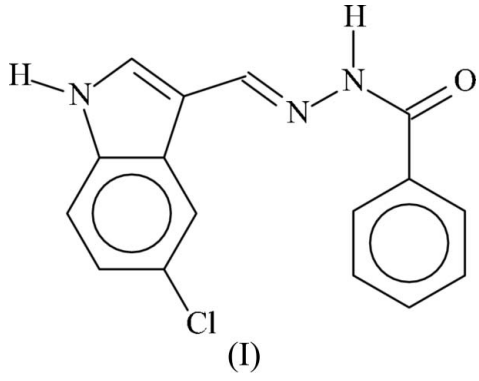
In the title compound, $C_{16}H_{12}ClN_3O$, the amide O atom serves as an N—H···O hydrogen-bond acceptor to the amide and amine groups of two adjacent molecules, resulting in a layered structure.

Comment

Previous studies on the Schiff bases derived by condensing 5-bromo-1*H*-indole-3-carbaldehyde with aroylhydrazines have described the 2-thienoylhydrazone (Ali *et al.*, 2005), the 2-nitrobenzoylhydrazone (Ali *et al.*, 2005*a*) and the 3-methoxybenzoylhydrazone (Ali *et al.*, 2005*b*) derivatives.



(I)

Here, these studies are extended to 5-chloro-1*H*-indole-3-carboxaldehyde, which has been condensed with benzhydrazine to give the title hydrazone, (I), (Fig. 1). Such compounds have long been known to have biological properties, e.g. *in vivo* monoamine oxidase-inhibiting activity (Alemany *et al.*, 1967).

The zigzag —C(O)—NH—N═CH— fragment in (I) has the attached 5-chloroindolyl portion of the molecule in a nearly coplanar conformation [dihedral angle = 9.4 (2)°]. However, the benzene ring attached to C10 is oriented away from it [dihedral angle = 53.2 (1)°], the twist being a compromise between crowding by H atoms and conjugation of the aromatic system along the length of the fragment. The moleculecrystal structurebonding; the amide O atom is an acceptor in two N—H···O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized by condensing 5-chloroindole-3-carbaldehyde (0.64 g, 3.5 mmol) with benzhydrazide (0.48 g, 3.5 mmol) in ethanol (100 ml). The solution was refluxed for 2 h. The solvent was removed and crystals of (I) were recrystallized from dimethylformamide.

Crystal data

$C_{16}H_{12}ClN_3O$
M_r = 297.74
Monoclinic, $P2_1/c$
a = 11.0860 (9) Å
b = 5.9337 (5) Å
c = 21.625 (2) Å
β = 95.336 (1)°
V = 1416.3 (2) Å^3
Z = 4
D_x = 1.396 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 295 (2) K
Block, yellow
0.34 × 0.30 × 0.24 mm

Data collection

Bruker APEX-II CCD diffractometer
ω scans
Absorption correction: none
12576 measured reflections
3131 independent reflections
2404 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 1.04
3131 reflections
198 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.2701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

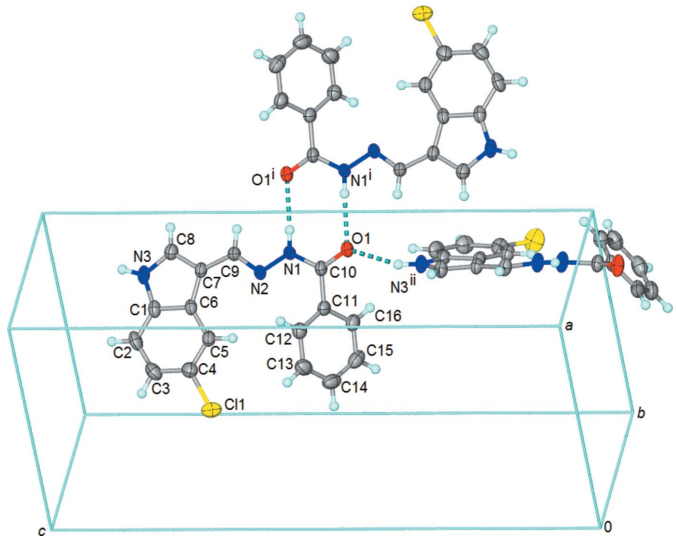


Figure 1
View of part of the packing of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. The dashed lines represent hydrogen bonds. [Symmetry codes: (i) $2-x, 2-y, 1-z$; (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$.]

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.86 (1)	2.10 (1)	2.950 (2)	172 (2)
N3—H3N···O1^{ii}	0.86 (1)	2.06 (1)	2.880 (2)	159 (2)

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

The carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C). The amide and amine H atoms were located in a difference Fourier map and were refined with the distance restraint N—H = 0.85 (1) Å; their U_{iso} values were 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*.

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