Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Bromo-1*H*-indole-3-carbaldehyde 3-methoxybenzoylhydrazone

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.114
Data-to-parameter ratio = 16.7

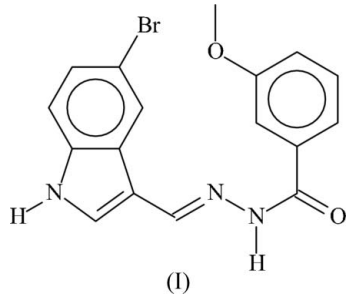
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 June 2005
Accepted 30 June 2005
Online 6 July 2005

Molecules of 5-bromo-1*H*-indole-3-carbaldehyde 3-methoxybenzoylylhydrazone, $C_{17}H_{14}BrN_3O_2$, are paired by amino–carbonyl hydrogen bonds over a center of inversion, and adjacent pairs are further linked by hydrogen bonds into ribbons.

Comment

Previous studies on the Schiff bases derived from 5-bromoindole-3-carbaldehyde include the thienoylhydrazone (Ali, Abdul Halim, Lajis *et al.*, 2005) and 2-nitrobenzoylhydrazone (Ali, Abdul Halim & Ng, 2005) derivatives. The 2-nitrobenzoylhydrazone derivative crystallizes as a hemihydrate, and the water molecule engages in hydrogen-bonding interactions, giving rise to a layer structure. The 3-methoxybenzoylhydrazone derivative, (I) (Fig. 1), reported here, is an anhydrous compound.



(I)

In the crystal structure, two molecules are linked by hydrogen bonds across a center of inversion, and adjacent pairs are further linked by hydrogen bonds into a ribbon motif (Fig. 2 and Table 1). The carbonyl O atom forms two hydrogen bonds.

Experimental

5-Bromoindole-3-carbaldehyde (0.40 g, 1.8 mmol) and 3-methoxybenzhydrazide (0.30 g, 1.8 mmol) were dissolved in a small volume of ethanol. The solution was heated for 2 h, after which time the solvent was removed to give the crude product which was purified by recrystallization from ethyl acetate.

Crystal data

$C_{17}H_{14}BrN_3O_2$
M_r = 372.22
Monoclinic, $C2/c$
a = 19.257 (4) Å
b = 8.904 (3) Å
c = 19.400 (4) Å
β = 108.330 (17)°
V = 3157.7 (13) Å^3
Z = 8
D_x = 1.566 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9770 reflections
θ = 3.1–27.5°
μ = 2.62 mm^{-1}
T = 295 (2) K
Block, brown
0.35 × 0.24 × 0.18 mm

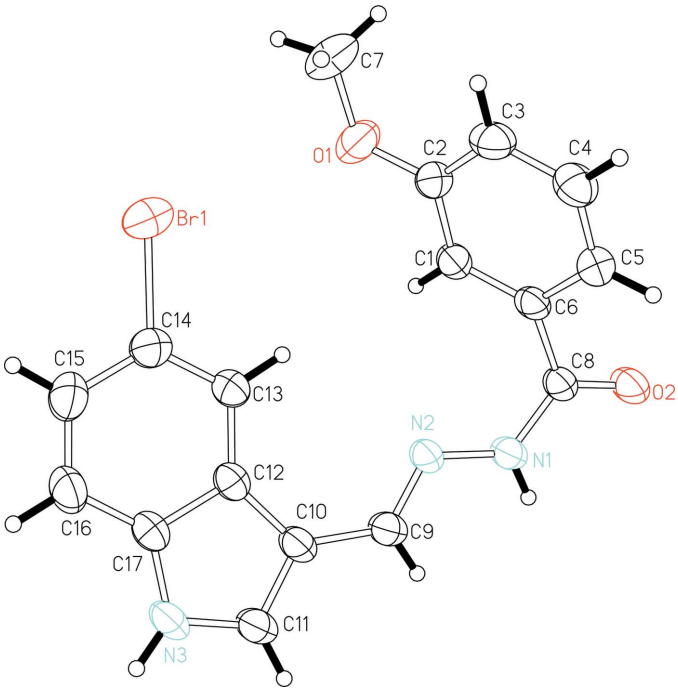


Figure 1
ORTEPII plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.315, T_{max} = 0.650
15076 measured reflections
3616 independent reflections
2664 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.5°
$h = -24 \rightarrow 23$
$k = -11 \rightarrow 11$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 1.08
3616 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 3.744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O2^{i}	0.87 (2)	2.15 (2)	3.010 (3)	170 (3)
N3—H3n···O2^{ii}	0.85 (2)	2.13 (2)	2.976 (3)	169 (3)

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

The aromatic H atoms were positioned geometrically (C—H = 0.93 Å) and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(parent atom). For the methyl H atoms (C—H = 0.96 Å), U_{iso}(H) = 1.5U_{eq}(C). The amino H atoms were located in a difference Fourier map and refined with a distance restraint of N—H = 0.85 (1) Å.

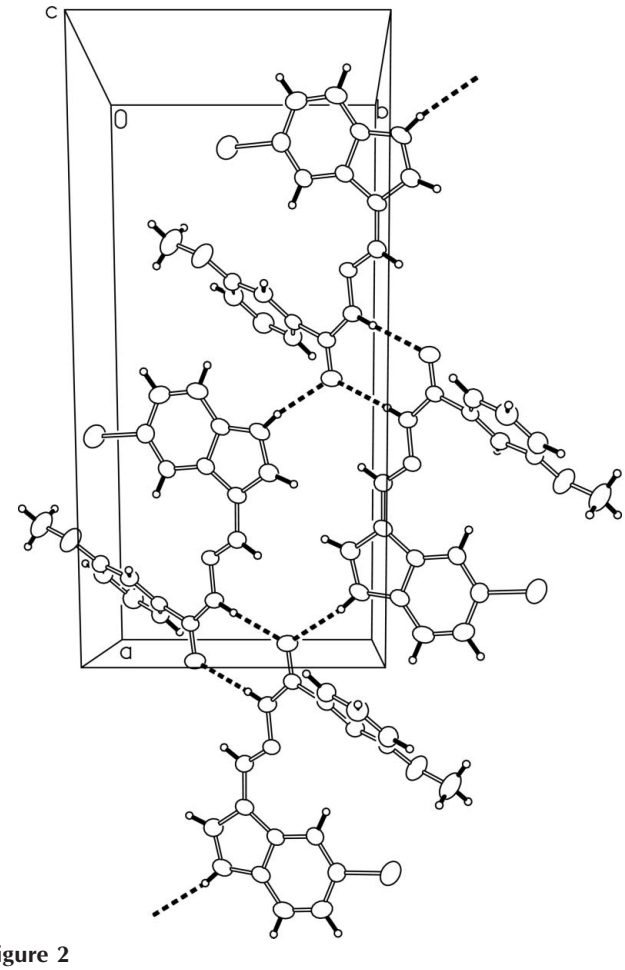


Figure 2
ORTEPII plot (Johnson, 1976) of the ribbon structure of (I). Hydrogen bonds are drawn as dashed lines.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the Ministry of Science, Technology and the Environment for supporting this study (grant No. IPRA 33–02-03–3055), and Professor Gao Shan of Heilongjiang University for carrying out the diffraction measurements.

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