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1*H*-Indole-3-carbaldehyde

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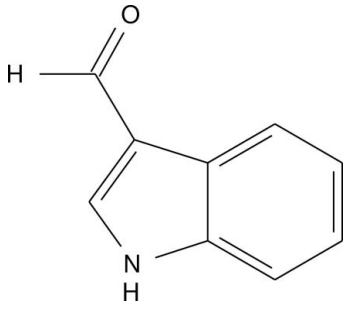
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.069; data-to-parameter ratio = 7.1.

In the title compound, C_9H_7NO, the benzene ring forms a dihedral angle of 3.98 (12)° with the pyrrole ring. In the crystal, N–H···O hydrogen bonds links the molecules into chains which run parallel to [02$\bar{1}$].

Related literature

For a related structure, see: Rizal *et al.* (2008).



Experimental

Crystal data

C_9H_7NO M_r = 145.16
Orthorhombic, $Pca2_1$
a = 14.0758 (9) Å
b = 5.8059 (4) Å
c = 8.6909 (5) Å
V = 710.24 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
3791 measured reflections
775 independent reflections
699 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
S = 1.08
775 reflections
109 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.09 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.94 (3)	1.92 (3)	2.831 (2)	165 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

CSD would like to acknowledge the UGC–BRS and the University of Mysore for financial asistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2070).

References

Bruker (2004). *APEX2*, *SAINT* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Rizal, M. R., Ali, H. M. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o555.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supporting information

Acta Cryst. (2012). E**68**, o3135 [doi:10.1107/S1600536812040573]

1*H*-Indole-3-carbaldehyde

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S1. Comment

The molecule is shown with its labelling in Figure 1. The molecules are connected into one-dimensional chains by the N1–H1A···O1(3/2-*x*,-1+*y*,1/2+*z* hydrogen bond which links the molecules into one dimensional chains which run parellel to [2-10], Table 1 and Figure2.

S2. Experimental

Indole was converted to 1*H*-indole-3-carbaldehyde in the presence of DMF, POCl3, NaOH. 1*H*-indole-3-carbaldehyde was taken and recrystallized in methanol solvent. The purity of the compound is confirmed by the TLC. A little quantity of compound was taken again for recrystallization to get a pure crystal in methanol solvent medium.

S3. Refinement

H atoms were treated as riding atoms with C—H(aromatic), 0.93 Å with U_{iso} = 1.2Ueq(C). The H atoms attached to C1 and N1 were located on a difference map and refined isotropically. Friedel pairs were merged.

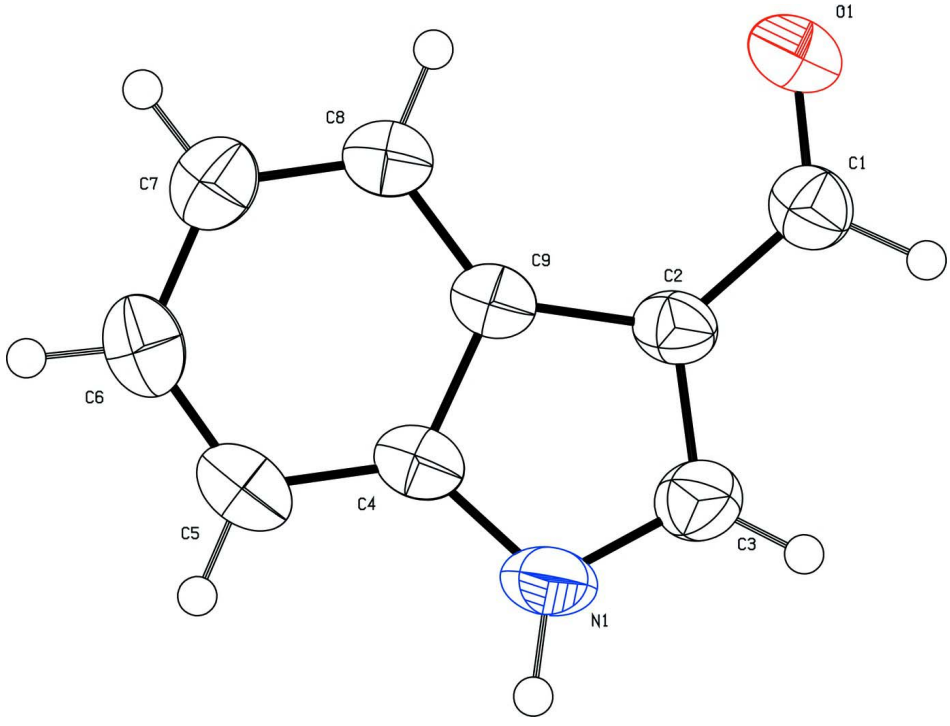

Figure 1

ORTEP of the title compound with the ellipsoids for non-H atoms are drawn at the 50% probability.

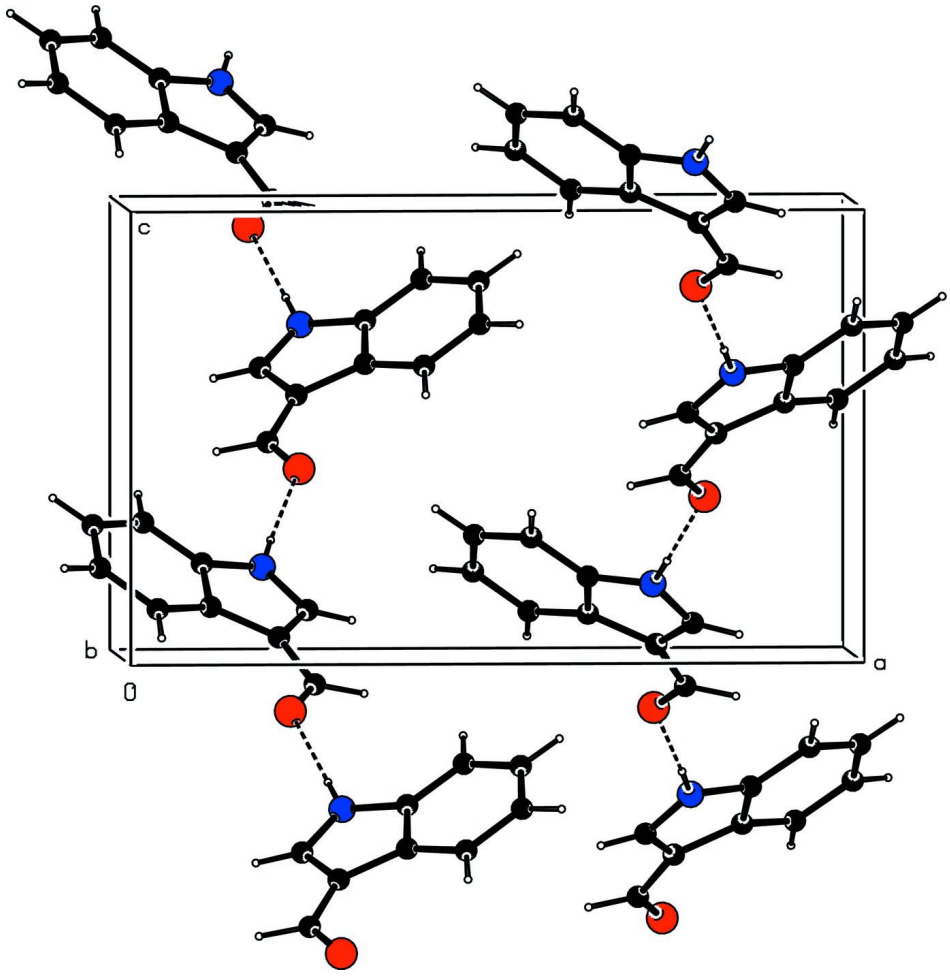

Figure 2

Molecular packing view of down the *b* axis. Dashed lines indicate hydrogen bonds.

1*H*-Indole-3-carbaldehyde

Crystal data

C_9H_7NO
$M_r = 145.16$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 14.0758\ (9)$ Å
$b = 5.8059\ (4)$ Å
$c = 8.6909\ (5)$ Å
$V = 710.24\ (8)$ Å^3
$Z = 4$
$F(000) = 304$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
3791 measured reflections

775 independent reflections
699 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.9°$
$h = -17 \rightarrow 16$
$k = -6 \rightarrow 7$
$l = -10 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.069$
$S = 1.08$
775 reflections
109 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 0.0895P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.09$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.031 (5)

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}
C1	0.76788 (16)	0.4092 (3)	−0.0642 (3)	0.0443 (5)
C2	0.72368 (14)	0.2453 (4)	0.0341 (3)	0.0401 (5)
C3	0.76781 (17)	0.0501 (4)	0.0871 (3)	0.0489 (6)
H3	0.8297	0.0074	0.0628	0.059*
C4	0.62446 (14)	0.0451 (3)	0.1907 (3)	0.0418 (5)
C5	0.54556 (17)	−0.0080 (4)	0.2797 (3)	0.0500 (6)
H5	0.5427	−0.1430	0.3371	0.060*
C6	0.47250 (16)	0.1462 (4)	0.2795 (3)	0.0535 (6)
H6	0.4189	0.1166	0.3388	0.064*
C7	0.47646 (15)	0.3467 (4)	0.1924 (3)	0.0526 (6)
H7	0.4255	0.4487	0.1951	0.063*
C8	0.55405 (16)	0.3976 (4)	0.1024 (3)	0.0449 (5)
H8	0.5555	0.5310	0.0433	0.054*
C9	0.63026 (14)	0.2450 (3)	0.1019 (2)	0.0370 (5)
N1	0.70988 (14)	−0.0700 (3)	0.1783 (2)	0.0510 (5)
O1	0.72964 (12)	0.5795 (2)	−0.1176 (2)	0.0565 (5)
H1	0.8360 (16)	0.376 (4)	−0.086 (3)	0.054 (6)*
H1A	0.7253 (17)	−0.204 (4)	0.233 (4)	0.073 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0516 (13)	0.0432 (10)	0.0382 (12)	−0.0002 (9)	0.0027 (11)	−0.0014 (10)
C2	0.0514 (11)	0.0368 (9)	0.0323 (10)	0.0032 (9)	0.0004 (9)	0.0009 (8)
C3	0.0557 (14)	0.0476 (11)	0.0435 (14)	0.0109 (11)	0.0050 (11)	0.0022 (10)
C4	0.0557 (12)	0.0341 (9)	0.0354 (11)	−0.0017 (8)	−0.0038 (10)	0.0013 (10)
C5	0.0666 (14)	0.0435 (12)	0.0399 (13)	−0.0135 (11)	−0.0021 (12)	0.0050 (10)
C6	0.0499 (13)	0.0624 (14)	0.0484 (14)	−0.0136 (11)	0.0036 (11)	−0.0011 (12)
C7	0.0466 (12)	0.0576 (13)	0.0536 (15)	0.0036 (10)	−0.0017 (12)	−0.0041 (14)
C8	0.0512 (12)	0.0406 (10)	0.0428 (13)	0.0013 (9)	−0.0046 (11)	0.0037 (9)
C9	0.0473 (11)	0.0344 (10)	0.0293 (10)	−0.0027 (8)	−0.0052 (9)	−0.0017 (8)
N1	0.0680 (12)	0.0395 (9)	0.0455 (11)	0.0102 (8)	0.0016 (10)	0.0113 (10)
O1	0.0658 (11)	0.0442 (8)	0.0596 (11)	−0.0002 (7)	0.0058 (8)	0.0163 (8)

Geometric parameters (Å, º)

C1—O1	1.218 (2)	C5—C6	1.363 (3)
C1—C2	1.422 (3)	C5—H5	0.9300
C1—H1	1.00 (2)	C6—C7	1.390 (3)
C2—C3	1.372 (3)	C6—H6	0.9300
C2—C9	1.441 (3)	C7—C8	1.375 (3)
C3—N1	1.334 (3)	C7—H7	0.9300
C3—H3	0.9300	C8—C9	1.391 (3)
C4—N1	1.380 (3)	C8—H8	0.9300
C4—C5	1.388 (3)	N1—H1A	0.94 (2)
C4—C9	1.396 (3)		
O1—C1—C2	125.4 (2)	C5—C6—C7	121.4 (2)
O1—C1—H1	120.6 (14)	C5—C6—H6	119.3
C2—C1—H1	114.0 (14)	C7—C6—H6	119.3
C3—C2—C1	123.8 (2)	C8—C7—C6	121.4 (2)
C3—C2—C9	105.93 (19)	C8—C7—H7	119.3
C1—C2—C9	130.22 (19)	C6—C7—H7	119.3
N1—C3—C2	110.8 (2)	C7—C8—C9	118.5 (2)
N1—C3—H3	124.6	C7—C8—H8	120.7
C2—C3—H3	124.6	C9—C8—H8	120.7
N1—C4—C5	129.30 (19)	C8—C9—C4	118.84 (19)
N1—C4—C9	107.95 (18)	C8—C9—C2	134.75 (19)
C5—C4—C9	122.65 (19)	C4—C9—C2	106.31 (18)
C6—C5—C4	117.2 (2)	C3—N1—C4	109.04 (17)
C6—C5—H5	121.4	C3—N1—H1A	126.4 (16)
C4—C5—H5	121.4	C4—N1—H1A	124.4 (16)
O1—C1—C2—C3	177.2 (2)	N1—C4—C9—C8	−176.6 (2)
O1—C1—C2—C9	−4.9 (4)	C5—C4—C9—C8	0.1 (3)
C1—C2—C3—N1	179.3 (2)	N1—C4—C9—C2	0.2 (2)
C9—C2—C3—N1	1.0 (3)	C5—C4—C9—C2	176.9 (2)

N1—C4—C5—C6	175.0 (2)	C3—C2—C9—C8	175.3 (2)
C9—C4—C5—C6	−0.9 (3)	C1—C2—C9—C8	−2.8 (4)
C4—C5—C6—C7	0.7 (4)	C3—C2—C9—C4	−0.7 (2)
C5—C6—C7—C8	0.3 (4)	C1—C2—C9—C4	−178.9 (2)
C6—C7—C8—C9	−1.1 (3)	C2—C3—N1—C4	−0.8 (3)
C7—C8—C9—C4	0.9 (3)	C5—C4—N1—C3	−176.0 (2)
C7—C8—C9—C2	−174.8 (2)	C9—C4—N1—C3	0.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.94 (3)	1.92 (3)	2.831 (2)	165 (3)

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