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2-Methyl-1-phenyl-1*H*-indole-3-carbonitrile

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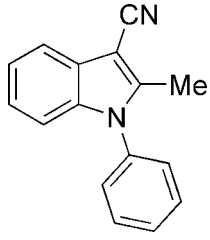
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.120; data-to-parameter ratio = 21.3.

In the title compound, $C_{16}H_{12}N_2$, the dihedral angle between the indole ring system and the pendant phenyl ring is 64.92 (5)°. The crystal packing features aromatic π–π stacking [centroid–centroid separation = 3.9504 (9) Å] and C—H$\cdots\pi$ interactions.

Related literature

For the synthesis of the title compound, see: Du *et al.* (2006). For its precursor, see: Jin *et al.* (2009). For related structures, see: Yang *et al.* (2011); Yan & Qi (2011*a*,*b*).



Experimental

Crystal data

$C_{16}H_{12}N_2$
M_r = 232.28
Triclinic, $P\overline{1}$
a = 6.3610 (5) Å
b = 9.497 (1) Å
c = 11.0210 (12) Å
α = 65.97 (2)°
β = 80.52 (2)°
γ = 88.13 (2)°
V = 599.34 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 K
0.26 × 0.24 × 0.06 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear-SM Expert*; Rigaku, 2009)
T_{min} = 0.980, T_{max} = 0.995
11425 measured reflections
3494 independent reflections
2309 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 0.98
3494 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*2 and *Cg*3 are the centroids of the C3–C8 and C11–C16 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C6—H6$\cdots$*Cg*3^{i}	0.95	2.85	3.719 (1)	152
C9—H9*A*$\cdots$*Cg*2^{ii}	0.98	2.94	3.799 (2)	147
C13—H13$\cdots$*Cg*2^{iii}	0.95	2.77	3.537 (2)	139

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

Data collection: *CrystalClear-SM Expert* (Rigaku 2009); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2009); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6411).

References

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supporting information

Acta Cryst. (2011). E**67**, o2902 [doi:10.1107/S1600536811039250]

2-Methyl-1-phenyl-1*H*-indole-3-carbonitrile

Kun Yang, Pei-Fan Li, Yan Liu and Zhi-Zhong Fang

S1. Comment

Indoles are an important compound possessing pharmaceutical properties. Extensive investigation on the crystal structures of indoles helps disclose their structure-activity relationship. For continuing our reseach, herein, we reported the crystal structure of the title indole derivative, (I).

In the molecular structure (Fig. 1), the components of the indole ring system are almost coplanar with a dihedral angle of 0.89 (7)° between its pyrrole part and benzene part. The indole ring forms an angle of 64.92 (5)° with the benzene ring.

In the molecular packing, π-π stacking and C—H···π interactions were observed, helping solidify the packing.

S2. Experimental

The title compound was prepared according to the method of the literature (Du *et al.*, 2006). Colourless prisms of (I) were grown from a mixture of ethyl actate and petroleum ether.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.95 and 0.98 Å)and refined as riding with U_{iso}(H) = 1.2U_{eq}(CH) or 1.5U_{eq}(CH_3).

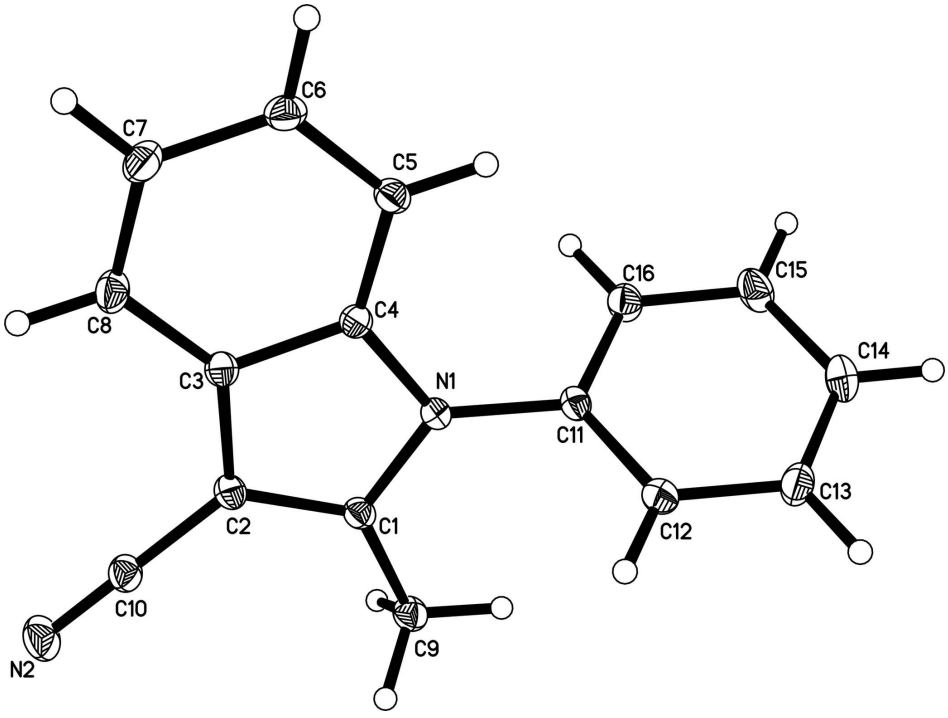

Figure 1

The molecular structure of (I) with 50% probability displacement ellipsoids.

2-Methyl-1-phenyl-1*H*-indole-3-carbonitrile

Crystal data

$C_{16}H_{12}N_2$
$M_r = 232.28$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.3610\ (5)$ Å
$b = 9.497\ (1)$ Å
$c = 11.0210\ (12)$ Å
$\alpha = 65.97\ (2)°$
$\beta = 80.52\ (2)°$
$\gamma = 88.13\ (2)°$
$V = 599.34\ (14)$ Å^3
$Z = 2$
$F(000) = 244$
$D_x = 1.287$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 2709 reflections
$\theta = 2.1–33.5°$
$\mu = 0.08$ mm^{-1}
$T = 113$ K
Prism, colorless
0.26 × 0.24 × 0.06 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.222 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*-SM Expert; Rigaku, 2009)
$T_{min} = 0.980$, $T_{max} = 0.995$
11425 measured reflections
3494 independent reflections
2309 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.1°$
$h = -8\rightarrow8$
$k = -13\rightarrow13$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.120$
$S = 0.98$
3494 reflections
164 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
$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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	0.44315 (14)	0.77239 (10)	0.77878 (9)	0.0185 (2)
N2	0.81470 (18)	0.84332 (13)	0.34779 (11)	0.0345 (3)
C1	0.60803 (17)	0.82767 (13)	0.67167 (11)	0.0194 (2)
C2	0.56979 (18)	0.77831 (13)	0.57514 (11)	0.0209 (2)
C3	0.37200 (18)	0.68851 (13)	0.62387 (11)	0.0202 (2)
C4	0.29646 (17)	0.68823 (12)	0.75088 (11)	0.0187 (2)
C5	0.10695 (18)	0.61245 (13)	0.82939 (11)	0.0216 (2)
H5	0.0582	0.6142	0.9150	0.026*
C6	−0.00823 (18)	0.53441 (14)	0.77872 (12)	0.0249 (3)
H6	−0.1391	0.4820	0.8299	0.030*
C7	0.06551 (19)	0.53158 (14)	0.65265 (12)	0.0275 (3)
H7	−0.0158	0.4763	0.6202	0.033*
C8	0.2539 (2)	0.60756 (14)	0.57463 (12)	0.0257 (3)
H8	0.3024	0.6049	0.4893	0.031*
C9	0.78658 (18)	0.92844 (14)	0.66577 (12)	0.0246 (3)
H9A	0.9227	0.8851	0.6449	0.030*
H9B	0.7777	0.9348	0.7530	0.030*
H9C	0.7772	1.0319	0.5955	0.030*
C10	0.70487 (19)	0.81451 (14)	0.44957 (12)	0.0240 (3)
C11	0.42676 (17)	0.78451 (12)	0.90546 (11)	0.0192 (2)
C12	0.57306 (19)	0.71355 (14)	0.98980 (12)	0.0248 (3)
H12	0.6857	0.6588	0.9629	0.030*
C13	0.5548 (2)	0.72252 (14)	1.11344 (12)	0.0285 (3)
H13	0.6578	0.6773	1.1701	0.034*
C14	0.3862 (2)	0.79746 (14)	1.15407 (12)	0.0293 (3)

H14	0.3723	0.8027	1.2393	0.035*
C15	0.2379 (2)	0.86476 (15)	1.07108 (12)	0.0313 (3)
H15	0.1207	0.9144	1.1002	0.038*
C16	0.25896 (19)	0.86032 (14)	0.94531 (12)	0.0261 (3)
H16	0.1589	0.9090	0.8873	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0180 (5)	0.0208 (5)	0.0170 (5)	0.0005 (4)	−0.0012 (3)	−0.0085 (4)
N2	0.0369 (6)	0.0412 (7)	0.0228 (5)	−0.0072 (5)	0.0039 (4)	−0.0131 (5)
C1	0.0185 (5)	0.0204 (5)	0.0174 (5)	0.0010 (4)	−0.0014 (4)	−0.0064 (4)
C2	0.0217 (6)	0.0224 (5)	0.0162 (5)	−0.0005 (4)	−0.0008 (4)	−0.0063 (4)
C3	0.0207 (6)	0.0209 (5)	0.0168 (5)	0.0004 (4)	−0.0029 (4)	−0.0054 (4)
C4	0.0187 (5)	0.0191 (5)	0.0177 (5)	0.0016 (4)	−0.0038 (4)	−0.0066 (4)
C5	0.0198 (6)	0.0236 (6)	0.0190 (5)	0.0003 (4)	−0.0006 (4)	−0.0071 (4)
C6	0.0198 (6)	0.0270 (6)	0.0247 (6)	−0.0036 (5)	−0.0030 (5)	−0.0072 (5)
C7	0.0279 (6)	0.0304 (6)	0.0253 (6)	−0.0051 (5)	−0.0080 (5)	−0.0108 (5)
C8	0.0306 (7)	0.0289 (6)	0.0178 (6)	−0.0019 (5)	−0.0056 (5)	−0.0089 (5)
C9	0.0235 (6)	0.0259 (6)	0.0228 (6)	−0.0043 (5)	0.0005 (4)	−0.0096 (5)
C10	0.0253 (6)	0.0261 (6)	0.0191 (6)	−0.0029 (5)	−0.0018 (4)	−0.0082 (5)
C11	0.0211 (5)	0.0191 (5)	0.0167 (5)	−0.0013 (4)	−0.0007 (4)	−0.0072 (4)
C12	0.0223 (6)	0.0291 (6)	0.0244 (6)	0.0048 (5)	−0.0032 (5)	−0.0127 (5)
C13	0.0323 (7)	0.0331 (7)	0.0220 (6)	0.0037 (5)	−0.0097 (5)	−0.0116 (5)
C14	0.0408 (8)	0.0278 (6)	0.0209 (6)	0.0001 (5)	−0.0030 (5)	−0.0121 (5)
C15	0.0363 (7)	0.0327 (7)	0.0267 (7)	0.0101 (6)	−0.0012 (5)	−0.0162 (5)
C16	0.0274 (6)	0.0287 (6)	0.0240 (6)	0.0086 (5)	−0.0059 (5)	−0.0123 (5)

Geometric parameters (Å, º)

N1—C1	1.3757 (14)	C7—H7	0.9500
N1—C4	1.3955 (14)	C8—H8	0.9500
N1—C11	1.4337 (13)	C9—H9A	0.9800
N2—C10	1.1514 (15)	C9—H9B	0.9800
C1—C2	1.3819 (16)	C9—H9C	0.9800
C1—C9	1.4853 (16)	C11—C16	1.3797 (16)
C2—C10	1.4183 (16)	C11—C12	1.3849 (16)
C2—C3	1.4398 (17)	C12—C13	1.3854 (16)
C3—C8	1.4006 (16)	C12—H12	0.9500
C3—C4	1.4020 (15)	C13—C14	1.3815 (17)
C4—C5	1.3877 (16)	C13—H13	0.9500
C5—C6	1.3804 (16)	C14—C15	1.3797 (17)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.4021 (17)	C15—C16	1.3881 (16)
C6—H6	0.9500	C15—H15	0.9500
C7—C8	1.3813 (17)	C16—H16	0.9500
C1—N1—C4	109.22 (9)	C3—C8—H8	120.7

C1—N1—C11	127.12 (9)	C1—C9—H9A	109.5
C4—N1—C11	123.45 (9)	C1—C9—H9B	109.5
N1—C1—C2	108.27 (10)	H9A—C9—H9B	109.5
N1—C1—C9	123.13 (10)	C1—C9—H9C	109.5
C2—C1—C9	128.56 (10)	H9A—C9—H9C	109.5
C1—C2—C10	124.37 (11)	H9B—C9—H9C	109.5
C1—C2—C3	108.35 (10)	N2—C10—C2	179.74 (14)
C10—C2—C3	127.28 (11)	C16—C11—C12	120.47 (10)
C8—C3—C4	119.01 (11)	C16—C11—N1	119.62 (10)
C8—C3—C2	135.08 (11)	C12—C11—N1	119.82 (10)
C4—C3—C2	105.90 (10)	C11—C12—C13	119.86 (11)
C5—C4—N1	129.20 (10)	C11—C12—H12	120.1
C5—C4—C3	122.53 (10)	C13—C12—H12	120.1
N1—C4—C3	108.27 (10)	C14—C13—C12	119.80 (11)
C6—C5—C4	117.64 (11)	C14—C13—H13	120.1
C6—C5—H5	121.2	C12—C13—H13	120.1
C4—C5—H5	121.2	C15—C14—C13	120.11 (11)
C5—C6—C7	120.81 (11)	C15—C14—H14	119.9
C5—C6—H6	119.6	C13—C14—H14	119.9
C7—C6—H6	119.6	C14—C15—C16	120.38 (11)
C8—C7—C6	121.36 (11)	C14—C15—H15	119.8
C8—C7—H7	119.3	C16—C15—H15	119.8
C6—C7—H7	119.3	C11—C16—C15	119.33 (11)
C7—C8—C3	118.63 (11)	C11—C16—H16	120.3
C7—C8—H8	120.7	C15—C16—H16	120.3

C4—N1—C1—C2	−0.61 (12)	C3—C4—C5—C6	0.38 (17)
C11—N1—C1—C2	174.22 (9)	C4—C5—C6—C7	0.39 (17)
C4—N1—C1—C9	177.02 (10)	C5—C6—C7—C8	−0.60 (18)
C11—N1—C1—C9	−8.15 (16)	C6—C7—C8—C3	0.03 (18)
N1—C1—C2—C10	179.25 (10)	C4—C3—C8—C7	0.71 (17)
C9—C1—C2—C10	1.79 (19)	C2—C3—C8—C7	179.55 (12)
N1—C1—C2—C3	0.15 (12)	C1—C2—C10—N2	113 (37)
C9—C1—C2—C3	−177.31 (11)	C3—C2—C10—N2	−68 (37)
C1—C2—C3—C8	−178.58 (13)	C1—N1—C11—C16	119.92 (13)
C10—C2—C3—C8	2.4 (2)	C4—N1—C11—C16	−65.94 (14)
C1—C2—C3—C4	0.36 (12)	C1—N1—C11—C12	−63.31 (15)
C10—C2—C3—C4	−178.71 (11)	C4—N1—C11—C12	110.84 (13)
C1—N1—C4—C5	−179.85 (11)	C16—C11—C12—C13	−1.93 (18)
C11—N1—C4—C5	5.09 (17)	N1—C11—C12—C13	−178.67 (10)
C1—N1—C4—C3	0.85 (12)	C11—C12—C13—C14	2.34 (19)
C11—N1—C4—C3	−174.22 (9)	C12—C13—C14—C15	−0.77 (19)
C8—C3—C4—C5	−0.94 (16)	C13—C14—C15—C16	−1.2 (2)
C2—C3—C4—C5	179.91 (10)	C12—C11—C16—C15	−0.06 (18)
C8—C3—C4—N1	178.42 (10)	N1—C11—C16—C15	176.69 (10)
C2—C3—C4—N1	−0.73 (12)	C14—C15—C16—C11	1.64 (19)
N1—C4—C5—C6	−178.84 (10)		

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C3–C8 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···*Cg*3^{i}	0.95	2.85	3.719 (1)	152
C9—H9*A*···*Cg*2^{ii}	0.98	2.94	3.799 (2)	147
C13—H13···*Cg*2^{iii}	0.95	2.77	3.537 (2)	139

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