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1-(4-Bromophenyl)-2-methyl-1*H*-indole-3-carbonitrile

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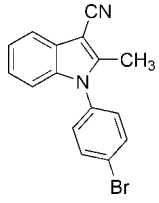
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.106; data-to-parameter ratio = 18.2.

In the title compound, $C_{16}H_{11}BrN_2$, the dihedral angle between the indole ring system and the phenyl ring is 58.85 (11)°.

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).



Experimental

Crystal data

$C_{16}H_{11}BrN_2$ M_r = 311.18
Monoclinic, $P2_1/n$
a = 9.170 (7) Å
b = 8.849 (6) Å
c = 16.337 (12) Å
β = 94.415 (15)°
V = 1321.7 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.10 mm^{-1}
T = 113 K
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2009)
T_{min} = 0.576, T_{max} = 0.671
12992 measured reflections
3147 independent reflections
2309 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.106
S = 1.00
3147 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6373).

References

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supporting information

Acta Cryst. (2011). E**67**, o2509 [doi:10.1107/S1600536811034246]

1-(4-Bromophenyl)-2-methyl-1*H*-indole-3-carbonitrile

Qiao Yan and Xiuxiang Qi

S1. Comment

In our continuing investigation of indole derivatives, herein, we reported the title compound (I). In the molecular structure,(Fig. 1), the indole ring is essentially planar with a dihedral angle of 0.95 (16)% between its pyrrole ring and fused benzene ring, similar to that [0.85 (6)°] of the 1-(2-chlorophenyl)- 6-fluoro-2-methyl-1*H*-indole-3-carbonitrile (Yang *et al.*, 2011), but less than that [2.66 (6)°] of our previously reported 1-(4-methoxyphenyl)-2-methyl-1*H*-indole-3-carbonitrile (Yan & Qi, 2011).

The indole ring constructs an angle of 58.85 (11) ° with the bromobenzene ring, similar to that [58.41 (4)°] reported by our group (Yan & Qi, 2011), but less than that [80.91 (5)°] reported by Yang *et al.* (2011). All the difference might be attributed to the steric substituent on the *N*-phenyl motif.

In the crystal packing, no significant π-π stacking interaction and C—H···π interaction were detected, unlike those reported in its anolog 1-(4-methoxyphenyl) -2-methyl-1*H*-indole-3-carbonitrile.

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).

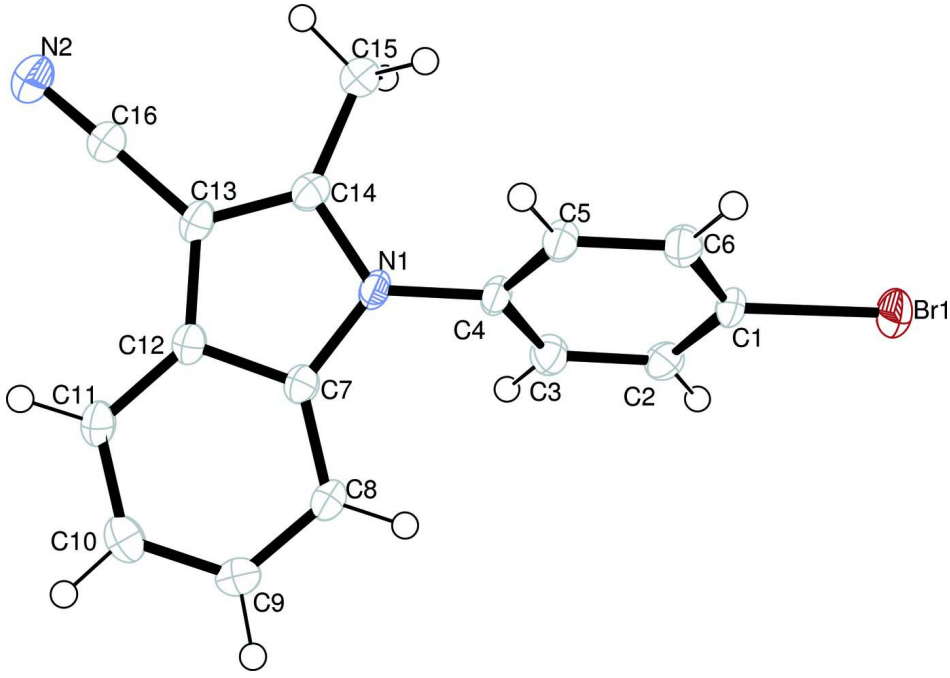

Figure 1

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

1-(4-Bromophenyl)-2-methyl-1*H*-indole-3-carbonitrile

Crystal data

$C_{16}H_{11}BrN_2$
$M_r = 311.18$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.170\ (7)$ Å
$b = 8.849\ (6)$ Å
$c = 16.337\ (12)$ Å
$\beta = 94.415\ (15)°$
$V = 1321.7\ (16)$ Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.564$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4781 reflections
$\theta = 2.2–27.9°$
$\mu = 3.10$ mm^{-1}
$T = 113$ K
Prism, colorless
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.22 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2009)
$T_{min} = 0.576$, $T_{max} = 0.671$
12992 measured reflections
3147 independent reflections
2309 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.5°$
$h = -12\rightarrow11$
$k = -11\rightarrow11$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.106$
$S = 1.00$
3147 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ 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}
Br1	1.31610 (4)	0.01069 (4)	0.08227 (2)	0.03260 (14)
N1	0.8376 (3)	0.4726 (3)	0.12974 (16)	0.0204 (6)
N2	0.3390 (3)	0.6165 (3)	0.11113 (18)	0.0341 (7)
C1	1.1681 (3)	0.1574 (3)	0.0968 (2)	0.0229 (7)
C2	1.1611 (4)	0.2252 (3)	0.1735 (2)	0.0248 (7)
H2	1.2302	0.2002	0.2178	0.030*
C3	1.0509 (4)	0.3301 (3)	0.18380 (19)	0.0243 (7)
H3	1.0444	0.3783	0.2354	0.029*
C4	0.9508 (3)	0.3642 (3)	0.11868 (19)	0.0205 (6)
C5	0.9610 (3)	0.2969 (3)	0.04233 (19)	0.0215 (7)
H5	0.8934	0.3230	−0.0024	0.026*
C6	1.0702 (3)	0.1913 (3)	0.0317 (2)	0.0236 (7)
H6	1.0770	0.1434	−0.0199	0.028*
C7	0.8620 (3)	0.6253 (3)	0.15065 (18)	0.0198 (6)
C8	0.9938 (3)	0.6992 (3)	0.17217 (18)	0.0225 (7)
H8	1.0846	0.6470	0.1749	0.027*
C9	0.9861 (4)	0.8520 (3)	0.18934 (19)	0.0250 (7)
H9	1.0732	0.9057	0.2058	0.030*
C10	0.8526 (4)	0.9285 (4)	0.18296 (19)	0.0264 (7)
H10	0.8513	1.0340	0.1938	0.032*
C11	0.7227 (4)	0.8555 (3)	0.16141 (18)	0.0236 (7)
H11	0.6327	0.9093	0.1574	0.028*
C12	0.7265 (3)	0.6991 (3)	0.14552 (18)	0.0206 (7)
C13	0.6191 (3)	0.5860 (3)	0.12233 (18)	0.0219 (7)
C14	0.6892 (3)	0.4497 (3)	0.11365 (19)	0.0218 (7)

C15	0.6229 (4)	0.2960 (3)	0.0985 (2)	0.0283 (8)
H15A	0.6327	0.2370	0.1494	0.042*
H15B	0.6736	0.2440	0.0560	0.042*
H15C	0.5190	0.3068	0.0803	0.042*
C16	0.4642 (4)	0.6019 (3)	0.11543 (19)	0.0245 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02374 (19)	0.0305 (2)	0.0430 (2)	0.01071 (15)	−0.00149 (15)	−0.00554 (15)
N1	0.0142 (12)	0.0235 (14)	0.0236 (14)	0.0045 (10)	0.0013 (11)	−0.0011 (10)
N2	0.0214 (16)	0.0380 (17)	0.0430 (18)	0.0044 (13)	0.0025 (14)	−0.0032 (13)
C1	0.0152 (15)	0.0197 (15)	0.0338 (18)	0.0052 (13)	0.0009 (13)	−0.0005 (13)
C2	0.0201 (16)	0.0257 (17)	0.0273 (17)	0.0019 (14)	−0.0059 (14)	0.0001 (13)
C3	0.0238 (17)	0.0261 (16)	0.0229 (17)	0.0023 (14)	0.0007 (14)	−0.0023 (12)
C4	0.0144 (15)	0.0214 (16)	0.0260 (16)	0.0040 (12)	0.0029 (13)	0.0004 (12)
C5	0.0185 (16)	0.0249 (16)	0.0211 (16)	0.0032 (13)	0.0018 (13)	−0.0012 (12)
C6	0.0219 (17)	0.0252 (16)	0.0238 (17)	0.0020 (13)	0.0017 (14)	−0.0027 (12)
C7	0.0184 (16)	0.0219 (16)	0.0194 (15)	0.0016 (13)	0.0031 (13)	−0.0001 (12)
C8	0.0164 (16)	0.0262 (17)	0.0249 (17)	0.0029 (13)	0.0021 (13)	0.0000 (12)
C9	0.0222 (18)	0.0271 (17)	0.0254 (17)	−0.0042 (14)	0.0004 (14)	0.0013 (13)
C10	0.0339 (19)	0.0220 (16)	0.0236 (17)	0.0031 (15)	0.0045 (15)	−0.0014 (12)
C11	0.0215 (17)	0.0245 (17)	0.0254 (17)	0.0059 (13)	0.0059 (14)	0.0000 (12)
C12	0.0190 (16)	0.0221 (16)	0.0211 (16)	0.0035 (13)	0.0039 (13)	0.0011 (12)
C13	0.0165 (15)	0.0259 (16)	0.0237 (16)	0.0034 (13)	0.0044 (13)	0.0022 (12)
C14	0.0180 (16)	0.0261 (16)	0.0216 (16)	−0.0003 (13)	0.0024 (13)	−0.0003 (12)
C15	0.0212 (17)	0.0278 (18)	0.036 (2)	0.0005 (14)	0.0003 (15)	−0.0058 (14)
C16	0.0201 (17)	0.0251 (17)	0.0283 (17)	0.0010 (14)	0.0019 (14)	−0.0014 (13)

Geometric parameters (Å, º)

Br1—C1	1.906 (3)	C7—C12	1.401 (4)
N1—C14	1.381 (4)	C8—C9	1.384 (4)
N1—C7	1.408 (4)	C8—H8	0.9500
N1—C4	1.435 (4)	C9—C10	1.396 (4)
N2—C16	1.152 (4)	C9—H9	0.9500
C1—C6	1.371 (4)	C10—C11	1.377 (4)
C1—C2	1.396 (4)	C10—H10	0.9500
C2—C3	1.393 (4)	C11—C12	1.410 (4)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.384 (4)	C12—C13	1.434 (4)
C3—H3	0.9500	C13—C14	1.379 (4)
C4—C5	1.392 (4)	C13—C16	1.423 (4)
C5—C6	1.391 (4)	C14—C15	1.503 (4)
C5—H5	0.9500	C15—H15A	0.9800
C6—H6	0.9500	C15—H15B	0.9800
C7—C8	1.395 (4)	C15—H15C	0.9800

C14—N1—C7	108.8 (2)	C7—C8—H8	121.6
C14—N1—C4	126.1 (3)	C8—C9—C10	121.1 (3)
C7—N1—C4	124.7 (3)	C8—C9—H9	119.4
C6—C1—C2	122.1 (3)	C10—C9—H9	119.4
C6—C1—Br1	118.8 (2)	C11—C10—C9	121.9 (3)
C2—C1—Br1	119.1 (2)	C11—C10—H10	119.1
C3—C2—C1	118.6 (3)	C9—C10—H10	119.1
C3—C2—H2	120.7	C10—C11—C12	118.3 (3)
C1—C2—H2	120.7	C10—C11—H11	120.8
C4—C3—C2	119.8 (3)	C12—C11—H11	120.8
C4—C3—H3	120.1	C7—C12—C11	118.7 (3)
C2—C3—H3	120.1	C7—C12—C13	106.2 (3)
C3—C4—C5	120.6 (3)	C11—C12—C13	135.1 (3)
C3—C4—N1	119.5 (3)	C14—C13—C16	123.2 (3)
C5—C4—N1	119.9 (3)	C14—C13—C12	108.8 (3)
C6—C5—C4	119.9 (3)	C16—C13—C12	127.8 (3)
C6—C5—H5	120.0	C13—C14—N1	108.2 (3)
C4—C5—H5	120.0	C13—C14—C15	128.5 (3)
C1—C6—C5	119.0 (3)	N1—C14—C15	123.0 (3)
C1—C6—H6	120.5	C14—C15—H15A	109.5
C5—C6—H6	120.5	C14—C15—H15B	109.5
C8—C7—C12	123.0 (3)	H15A—C15—H15B	109.5
C8—C7—N1	129.0 (3)	C14—C15—H15C	109.5
C12—C7—N1	108.0 (3)	H15A—C15—H15C	109.5
C9—C8—C7	116.9 (3)	H15B—C15—H15C	109.5
C9—C8—H8	121.6	N2—C16—C13	178.7 (4)

C6—C1—C2—C3	0.1 (5)	C9—C10—C11—C12	0.0 (5)
Br1—C1—C2—C3	−178.9 (2)	C8—C7—C12—C11	1.1 (5)
C1—C2—C3—C4	0.4 (5)	N1—C7—C12—C11	−178.1 (3)
C2—C3—C4—C5	−1.4 (5)	C8—C7—C12—C13	−179.8 (3)
C2—C3—C4—N1	−179.9 (3)	N1—C7—C12—C13	1.0 (3)
C14—N1—C4—C3	−125.7 (3)	C10—C11—C12—C7	−1.3 (4)
C7—N1—C4—C3	61.5 (4)	C10—C11—C12—C13	179.9 (3)
C14—N1—C4—C5	55.8 (4)	C7—C12—C13—C14	−0.3 (3)
C7—N1—C4—C5	−117.1 (3)	C11—C12—C13—C14	178.6 (3)
C3—C4—C5—C6	1.7 (5)	C7—C12—C13—C16	174.7 (3)
N1—C4—C5—C6	−179.7 (3)	C11—C12—C13—C16	−6.4 (6)
C2—C1—C6—C5	0.2 (5)	C16—C13—C14—N1	−175.8 (3)
Br1—C1—C6—C5	179.2 (2)	C12—C13—C14—N1	−0.6 (3)
C4—C5—C6—C1	−1.1 (5)	C16—C13—C14—C15	−2.0 (5)
C14—N1—C7—C8	179.4 (3)	C12—C13—C14—C15	173.2 (3)
C4—N1—C7—C8	−6.7 (5)	C7—N1—C14—C13	1.2 (3)
C14—N1—C7—C12	−1.4 (3)	C4—N1—C14—C13	−172.6 (3)
C4—N1—C7—C12	172.5 (3)	C7—N1—C14—C15	−173.0 (3)
C12—C7—C8—C9	0.4 (5)	C4—N1—C14—C15	13.2 (5)
N1—C7—C8—C9	179.5 (3)	C14—C13—C16—N2	136 (18)
C7—C8—C9—C10	−1.8 (5)	C12—C13—C16—N2	−38 (18)

C8—C9—C10—C11	1.6 (5)