Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(7-Methyl-1*H*-indol-3-yl)acetonitrile

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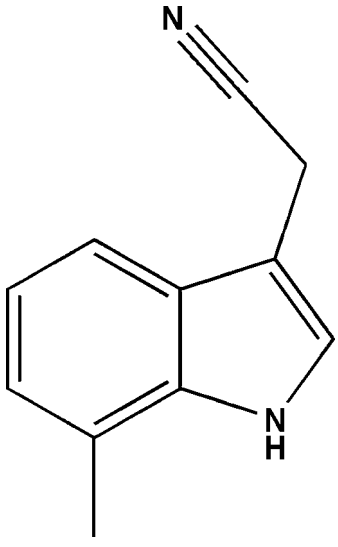
Received 1 December 2011; accepted 12 December 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.154; data-to-parameter ratio = 18.3.

In the title compound, $C_{11}H_{10}N_2$, the carbonitrile group is twisted away from the indole plane [$C_{cy}—C_{me}—C_{ar}—C_{ar}$ = 66.6 (2)°; cy = cyanide, me = methylene and ar = aromatic]. In the crystal, N—H···N hydrogen bonds link the molecules into $C(7)$ chains propagating in the [001] direction.

Related literature

For background to indole derivatives as pharmaceuticals, see: Kunzer & Wendt (2011).



Experimental

Crystal data

$C_{11}H_{10}N_2$
M_r = 170.21
Monoclinic, $P2_1/c$
a = 6.9962 (14) Å
b = 8.9445 (18) Å
c = 15.406 (3) Å
β = 97.97 (3)°
V = 954.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 K
0.26 × 0.24 × 0.15 mm

Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.981, T_{max} = 0.989
9402 measured reflections
2160 independent reflections
1418 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.154
S = 1.05
2160 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.86	2.24	3.022 (2)	151

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

We thank Southeast University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6546).

References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Kunzer, A. R. & Wendt, M. D. (2011). *Tetrahedron*, **52**, 1815–1818.
Rigaku. (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
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supporting information

Acta Cryst. (2012). E**68**, o141 [doi:10.1107/S1600536811053396]

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S1. Experimental

Colourless blocks of (I) were obstained by slow evaporation of a methanol solution of a commercially supplied sample.

S2. Refinement

All H atoms attached to C atoms and O atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH), C—H = 0.97 Å (CH_2), C—H = 0.96 Å (CH_3)and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(CH, CH_2 and NH) and U_{iso}(H) = 1.5U_{eq}(CH_3).

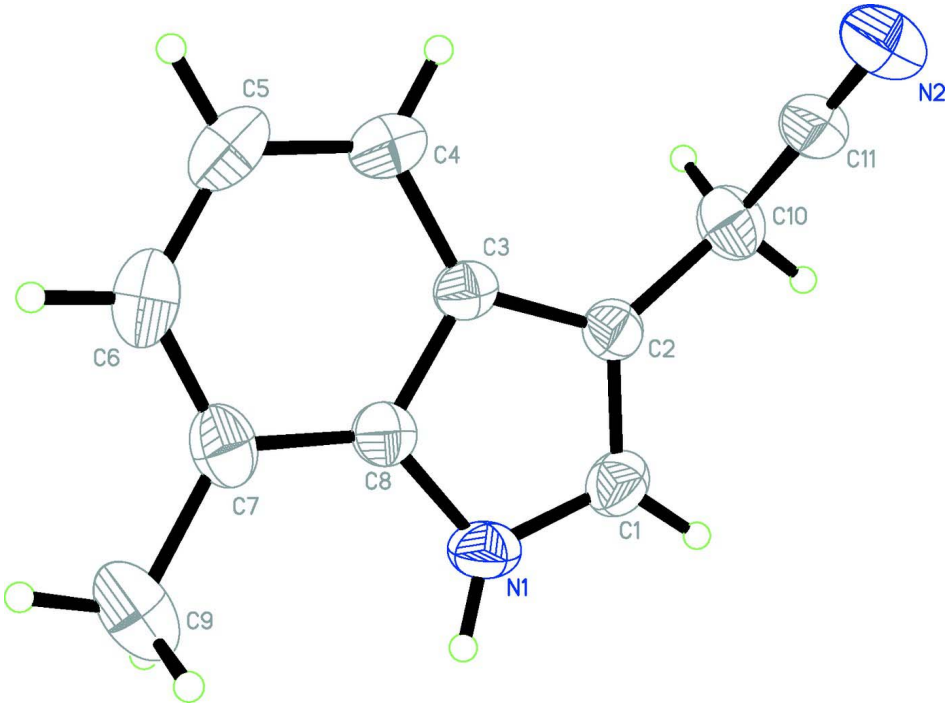

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

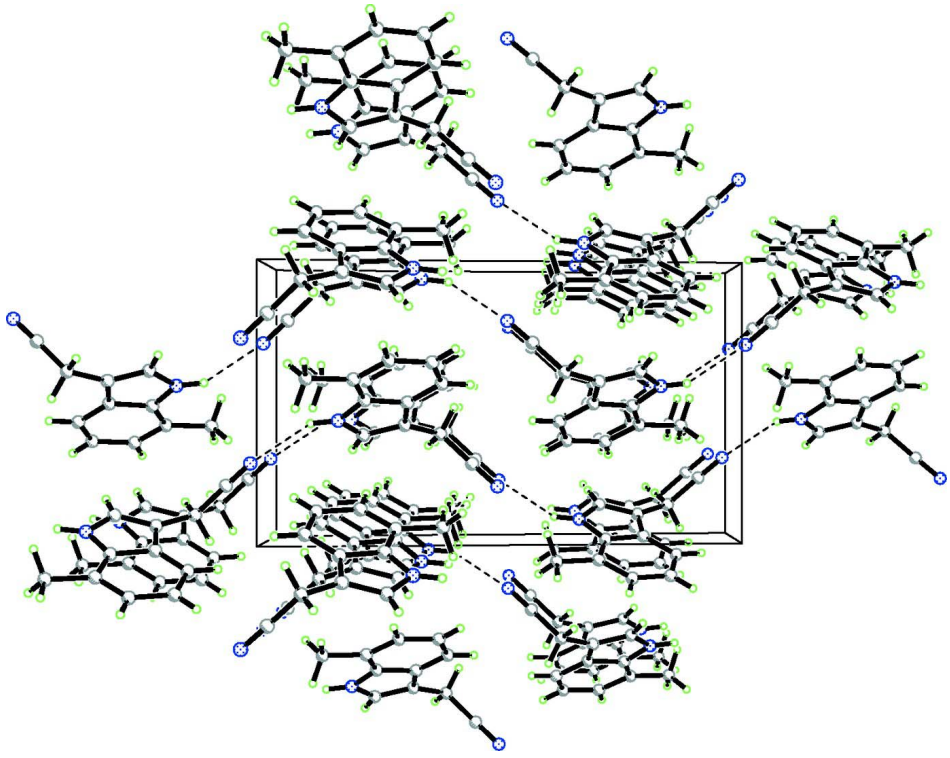

Figure 2

A packing view down the *a* axis with hydrogen bonds shown as dashed lines.

2-(7-Methyl-1*H*-indol-3-yl)acetonitrile

Crystal data

$C_{11}H_{10}N_2$
$M_r = 170.21$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.9962\ (14)$ Å
$b = 8.9445\ (18)$ Å
$c = 15.406\ (3)$ Å
$\beta = 97.97\ (3)°$
$V = 954.7\ (3)$ Å^3
$Z = 4$
$F(000) = 360$
$D_x = 1.184$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2175 reflections
$\theta = 2.7–27.5°$
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Block, colourless
0.26 × 0.24 × 0.15 mm

Data collection

Rigaku SCXmini CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.981$, $T_{max} = 0.989$
9402 measured reflections
2160 independent reflections
1418 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -9\rightarrow9$
$k = -11\rightarrow11$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.154$
$S = 1.05$
2160 reflections
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 0.0707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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}
C1	−0.0179 (3)	0.6121 (2)	0.21424 (12)	0.0587 (5)
H1B	−0.1278	0.6642	0.1903	0.070*
C2	0.0270 (2)	0.57655 (18)	0.30000 (11)	0.0511 (4)
C3	0.2072 (2)	0.49843 (17)	0.30912 (10)	0.0473 (4)
C4	0.3276 (3)	0.43296 (19)	0.37953 (12)	0.0613 (5)
H4A	0.2955	0.4369	0.4361	0.074*
C5	0.4936 (3)	0.3631 (2)	0.36311 (16)	0.0758 (6)
H5A	0.5736	0.3187	0.4092	0.091*
C6	0.5451 (3)	0.3571 (2)	0.27861 (17)	0.0768 (6)
H6A	0.6588	0.3088	0.2703	0.092*
C7	0.4334 (3)	0.4204 (2)	0.20730 (13)	0.0644 (5)
C8	0.2629 (2)	0.48979 (17)	0.22467 (10)	0.0506 (4)
C9	0.4896 (4)	0.4170 (3)	0.11583 (16)	0.0958 (8)
H9A	0.6091	0.3639	0.1168	0.144*
H9B	0.5047	0.5175	0.0959	0.144*
H9C	0.3905	0.3676	0.0768	0.144*
C10	−0.0948 (3)	0.6089 (2)	0.37116 (13)	0.0678 (5)
H10A	−0.2171	0.6509	0.3449	0.081*
H10B	−0.1216	0.5158	0.3994	0.081*
C11	−0.0021 (3)	0.7128 (2)	0.43771 (12)	0.0621 (5)
N1	0.1212 (2)	0.56067 (16)	0.16799 (9)	0.0600 (4)
H1A	0.1207	0.5707	0.1124	0.072*
N2	0.0698 (3)	0.7913 (2)	0.48993 (11)	0.0856 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0586 (10)	0.0557 (10)	0.0580 (11)	0.0065 (8)	−0.0048 (9)	−0.0008 (8)
C2	0.0529 (9)	0.0500 (9)	0.0495 (10)	0.0010 (7)	0.0040 (7)	−0.0038 (7)
C3	0.0537 (9)	0.0413 (8)	0.0454 (9)	−0.0049 (7)	0.0021 (7)	0.0014 (6)
C4	0.0659 (11)	0.0584 (11)	0.0562 (10)	−0.0058 (9)	−0.0030 (9)	0.0094 (8)
C5	0.0656 (12)	0.0597 (12)	0.0951 (16)	0.0036 (10)	−0.0131 (11)	0.0164 (11)
C6	0.0601 (12)	0.0574 (12)	0.1126 (18)	0.0064 (9)	0.0108 (12)	−0.0067 (12)
C7	0.0642 (11)	0.0542 (11)	0.0780 (13)	−0.0045 (9)	0.0207 (10)	−0.0131 (9)
C8	0.0585 (10)	0.0425 (9)	0.0503 (9)	−0.0045 (7)	0.0055 (8)	−0.0040 (7)
C9	0.0977 (17)	0.0985 (17)	0.1011 (18)	−0.0132 (14)	0.0481 (14)	−0.0277 (13)
C10	0.0606 (11)	0.0731 (12)	0.0715 (12)	−0.0027 (9)	0.0156 (10)	−0.0097 (10)
C11	0.0675 (11)	0.0716 (12)	0.0490 (10)	0.0085 (10)	0.0150 (9)	0.0013 (9)
N1	0.0748 (10)	0.0628 (9)	0.0404 (8)	−0.0020 (8)	0.0012 (7)	0.0008 (6)
N2	0.1026 (14)	0.0986 (14)	0.0549 (10)	0.0050 (11)	0.0087 (9)	−0.0152 (9)

Geometric parameters (Å, º)

C1—C2	1.353 (2)	C6—H6A	0.9300
C1—N1	1.364 (2)	C7—C8	1.403 (2)
C1—H1B	0.9300	C7—C9	1.515 (3)
C2—C3	1.431 (2)	C8—N1	1.381 (2)
C2—C10	1.507 (2)	C9—H9A	0.9600
C3—C4	1.405 (2)	C9—H9B	0.9600
C3—C8	1.411 (2)	C9—H9C	0.9600
C4—C5	1.373 (3)	C10—C11	1.467 (3)
C4—H4A	0.9300	C10—H10A	0.9700
C5—C6	1.399 (3)	C10—H10B	0.9700
C5—H5A	0.9300	C11—N2	1.131 (2)
C6—C7	1.378 (3)	N1—H1A	0.8600
C2—C1—N1	110.17 (15)	C8—C7—C9	121.5 (2)
C2—C1—H1B	124.9	N1—C8—C7	129.60 (17)
N1—C1—H1B	124.9	N1—C8—C3	106.97 (15)
C1—C2—C3	107.04 (15)	C7—C8—C3	123.43 (17)
C1—C2—C10	125.94 (16)	C7—C9—H9A	109.5
C3—C2—C10	126.99 (15)	C7—C9—H9B	109.5
C4—C3—C8	118.43 (16)	H9A—C9—H9B	109.5
C4—C3—C2	134.80 (16)	C7—C9—H9C	109.5
C8—C3—C2	106.76 (14)	H9A—C9—H9C	109.5
C5—C4—C3	118.63 (18)	H9B—C9—H9C	109.5
C5—C4—H4A	120.7	C11—C10—C2	112.97 (15)
C3—C4—H4A	120.7	C11—C10—H10A	109.0
C4—C5—C6	121.50 (19)	C2—C10—H10A	109.0
C4—C5—H5A	119.2	C11—C10—H10B	109.0
C6—C5—H5A	119.2	C2—C10—H10B	109.0
C7—C6—C5	122.37 (19)	H10A—C10—H10B	107.8

C7—C6—H6A	118.8	N2—C11—C10	179.0 (2)
C5—C6—H6A	118.8	C1—N1—C8	109.06 (14)
C6—C7—C8	115.63 (18)	C1—N1—H1A	125.5
C6—C7—C9	122.82 (19)	C8—N1—H1A	125.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{i}	0.86	2.24	3.022 (2)	151

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