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2-(4-Methoxy-1*H*-indol-3-yl)acetonitrile

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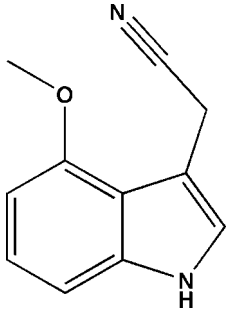
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.088; wR factor = 0.298; data-to-parameter ratio = 18.0.

In the title compound, $C_{11}H_{10}N_2O$, the cyanide group is twisted away from the indole-ring plane [$C_{cy}-C_{me}-C_{ar}-C_{ar}$ = 70.7 (2)°; cy = cyanide, me = methylene, ar = aromatic], whereas the methoxy C atom is almost coplanar with the ring system [displacement = 0.014 (5) Å]. In the crystal, N—H···N hydrogen bonds link the molecules into $C(7)$ chains propagating in [100].

Related literature

For a related structure, see: Ge *et al.* (2012).



Experimental

Crystal data

$C_{11}H_{10}N_2O$ M_r = 186.21
Monoclinic, $P2_1/c$
a = 8.3182 (17) Å
b = 13.062 (3) Å
c = 9.3867 (19) Å
β = 101.53 (3)°
V = 999.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 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} = 0.979, T_{max} = 0.988
9998 measured reflections
2283 independent reflections
1235 reflections with $I > 2\sigma(I)$
R_{int} = 0.109

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.088
$wR(F^2)$ = 0.298
S = 1.07
2283 reflections
127 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 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	2.19	3.028 (4)	164

Symmetry code: (i) $x+1, y, z$.

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: HB6547).

References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
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Rigaku. (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o143 [doi:10.1107/S1600536811053360]

2-(4-Methoxy-1*H*-indol-3-yl)acetonitrile

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S1. Experimental

Colourless blocks of the title compound, obtained from a commercial source, were obtained by slow evaporation of a methanol solution.

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).

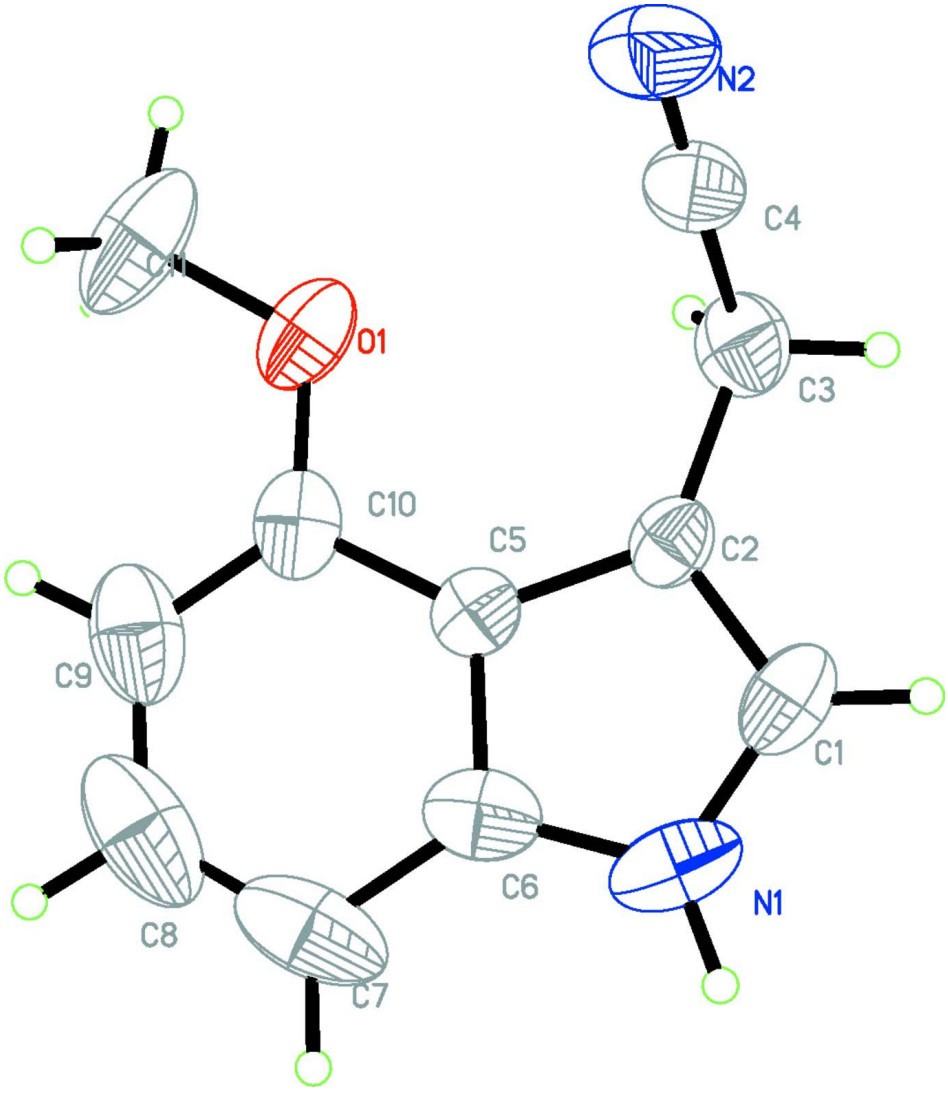

Figure 1

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

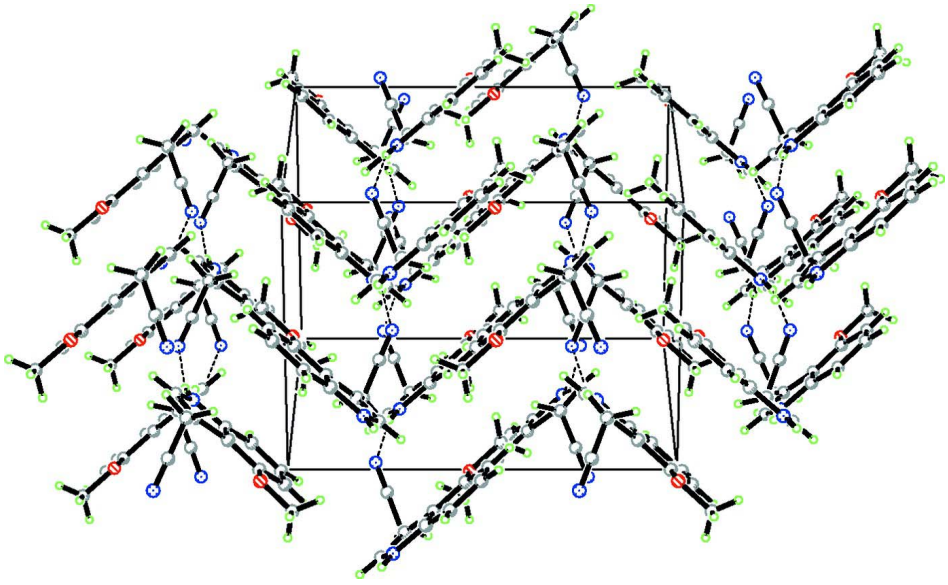

Figure 2

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

2-(4-Methoxy-1*H*-indol-3-yl)acetonitrile

Crystal data

$C_{11}H_{10}N_2O$
$M_r = 186.21$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.3182\ (17)$ Å
$b = 13.062\ (3)$ Å
$c = 9.3867\ (19)$ Å
$\beta = 101.53\ (3)°$
$V = 999.3\ (3)$ Å^3
$Z = 4$
$F(000) = 392$
$D_x = 1.238$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2283 reflections
$\theta = 3.1–27.5°$
$\mu = 0.08$ 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
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.979$, $T_{max} = 0.988$
9998 measured reflections
2283 independent reflections
1235 reflections with $I > 2\sigma(I)$
$R_{int} = 0.109$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -10\rightarrow10$
$k = -16\rightarrow16$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.088$
$wR(F^2) = 0.298$
$S = 1.07$
2283 reflections
127 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.1429P)^2 + 0.1759P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ 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}
C5	0.4959 (3)	0.6202 (2)	0.1157 (3)	0.0567 (7)
C2	0.4374 (4)	0.6934 (2)	0.0033 (3)	0.0610 (8)
C10	0.4215 (5)	0.5425 (2)	0.1837 (3)	0.0724 (9)
O1	0.2566 (3)	0.53144 (18)	0.1335 (3)	0.0941 (9)
N1	0.7052 (4)	0.7163 (3)	0.0794 (4)	0.0927 (11)
H1A	0.8020	0.7415	0.0864	0.111*
C6	0.6656 (4)	0.6374 (3)	0.1600 (4)	0.0770 (10)
N2	0.0524 (4)	0.7726 (3)	0.0570 (4)	0.0978 (11)
C4	0.1475 (4)	0.7424 (3)	−0.0049 (4)	0.0760 (10)
C1	0.5681 (5)	0.7495 (3)	−0.0147 (4)	0.0811 (10)
H1B	0.5653	0.8027	−0.0810	0.097*
C3	0.2684 (4)	0.7039 (3)	−0.0858 (3)	0.0806 (10)
H3A	0.2720	0.7501	−0.1661	0.097*
H3B	0.2323	0.6376	−0.1266	0.097*
C9	0.5176 (6)	0.4845 (3)	0.2916 (5)	0.1116 (12)
H9A	0.4708	0.4329	0.3382	0.134*
C7	0.7644 (6)	0.5791 (3)	0.2705 (4)	0.1120 (12)
H7A	0.8762	0.5912	0.3007	0.134*
C8	0.6861 (6)	0.5044 (4)	0.3297 (5)	0.1123 (11)
H8A	0.7486	0.4634	0.4008	0.135*
C11	0.1740 (7)	0.4533 (4)	0.1992 (6)	0.141 (2)
H11A	0.0594	0.4535	0.1553	0.212*
H11B	0.1872	0.4664	0.3015	0.212*
H11C	0.2203	0.3877	0.1846	0.212*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C5	0.0627 (17)	0.0571 (15)	0.0523 (15)	−0.0009 (12)	0.0163 (12)	−0.0114 (12)
C2	0.0707 (18)	0.0654 (17)	0.0507 (15)	−0.0105 (13)	0.0213 (13)	−0.0056 (13)
C10	0.099 (2)	0.0579 (17)	0.0641 (19)	0.0040 (16)	0.0265 (18)	−0.0044 (13)
O1	0.107 (2)	0.0782 (16)	0.1058 (19)	−0.0287 (13)	0.0425 (16)	0.0047 (13)

N1	0.0673 (18)	0.104 (2)	0.116 (3)	−0.0194 (16)	0.0396 (18)	−0.041 (2)
C6	0.074 (2)	0.082 (2)	0.077 (2)	0.0092 (17)	0.0204 (17)	−0.0287 (18)
N2	0.0590 (17)	0.125 (3)	0.104 (3)	−0.0091 (17)	0.0054 (17)	−0.009 (2)
C4	0.0611 (19)	0.089 (2)	0.071 (2)	−0.0100 (17)	−0.0037 (16)	0.0014 (17)
C1	0.097 (3)	0.077 (2)	0.082 (2)	−0.0183 (18)	0.048 (2)	−0.0083 (17)
C3	0.086 (2)	0.098 (2)	0.0561 (18)	−0.0022 (18)	0.0085 (16)	0.0000 (16)
C9	0.146 (2)	0.0971 (19)	0.0851 (18)	0.054 (2)	0.0086 (18)	−0.0107 (15)
C7	0.140 (3)	0.102 (2)	0.0871 (18)	0.058 (2)	0.0063 (18)	−0.0196 (15)
C8	0.145 (2)	0.0994 (19)	0.0859 (17)	0.059 (2)	0.0063 (17)	−0.0142 (14)
C11	0.195 (5)	0.090 (3)	0.167 (5)	−0.063 (3)	0.105 (4)	−0.013 (3)

Geometric parameters (Å, º)

C5—C6	1.407 (4)	C4—C3	1.465 (6)
C5—C10	1.407 (4)	C1—H1B	0.9300
C5—C2	1.435 (4)	C3—H3A	0.9700
C2—C1	1.350 (4)	C3—H3B	0.9700
C2—C3	1.492 (4)	C9—C8	1.400 (7)
C10—O1	1.365 (4)	C9—H9A	0.9300
C10—C9	1.384 (5)	C7—C8	1.353 (7)
O1—C11	1.437 (4)	C7—H7A	0.9300
N1—C6	1.357 (5)	C8—H8A	0.9300
N1—C1	1.366 (5)	C11—H11A	0.9600
N1—H1A	0.8600	C11—H11B	0.9600
C6—C7	1.411 (5)	C11—H11C	0.9600
N2—C4	1.142 (5)		
C6—C5—C10	119.2 (3)	C4—C3—H3A	108.7
C6—C5—C2	106.4 (3)	C2—C3—H3A	108.7
C10—C5—C2	134.3 (3)	C4—C3—H3B	108.7
C1—C2—C5	106.9 (3)	C2—C3—H3B	108.7
C1—C2—C3	124.9 (3)	H3A—C3—H3B	107.6
C5—C2—C3	128.1 (3)	C10—C9—C8	119.2 (5)
O1—C10—C9	126.0 (4)	C10—C9—H9A	120.4
O1—C10—C5	115.0 (3)	C8—C9—H9A	120.4
C9—C10—C5	119.0 (4)	C8—C7—C6	115.7 (5)
C10—O1—C11	117.4 (4)	C8—C7—H7A	122.2
C6—N1—C1	109.7 (3)	C6—C7—H7A	122.2
C6—N1—H1A	125.2	C9—C8—C7	124.7 (4)
C1—N1—H1A	125.2	C9—C8—H8A	117.6
N1—C6—C5	107.3 (3)	C7—C8—H8A	117.6
N1—C6—C7	130.4 (4)	O1—C11—H11A	109.5
C5—C6—C7	122.2 (4)	O1—C11—H11B	109.5
N2—C4—C3	179.4 (4)	H11A—C11—H11B	109.5
C2—C1—N1	109.6 (3)	O1—C11—H11C	109.5
C2—C1—H1B	125.2	H11A—C11—H11C	109.5
N1—C1—H1B	125.2	H11B—C11—H11C	109.5
C4—C3—C2	114.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{i}	0.86	2.19	3.028 (4)	164

Symmetry code: (i) *x*+1, *y*, *z*.