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1-Methoxy-2-methyl-1*H*-benzo[*f*]indole-3-carbonitrile

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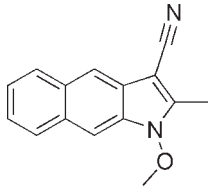
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.094; data-to-parameter ratio = 12.4.

Apart from the methyl group of the methoxy fragment, the title compound, $C_{15}H_{12}N_2O$, is almost planar (r.m.s. deviation = 0.045 Å); the C atom deviates from the mean plane by 1.216 (1) Å. In the crystal, π–π stacking [shortest centroid–centroid separation = 3.4652 (10) Å] and C—H$\cdots\pi$ interactions occur.

Related literature

For the synthesis, see: Du *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{12}N_2O$ M_r = 236.27
Monoclinic, $C2/c$
a = 18.663 (4) Å
b = 7.3763 (15) Å
c = 18.589 (4) Å
β = 113.46 (3)°
V = 2347.6 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 113 K
0.20 × 0.18 × 0.16 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.983, T_{max} = 0.986
11412 measured reflections
2060 independent reflections
1858 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.04
2060 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

*Cg*3 is the centroid of the C4–C9 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots$*Cg*3^{i}	0.93	2.65	3.3956 (15)	138

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

Data collection: *CrystalClear* (Rigaku/MSC, 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5274).

References

Du, Y. F., Chang, J. B., Reiner, J. & Zhao, K. (2008). *J. Org. Chem.* **73**, 2007–2010.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o97 [**doi:10.1107/S1600536809052416**]

1-Methoxy-2-methyl-1*H*-benzo[*f*]indole-3-carbonitrile

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Comment

The title compound, (I), comprises of a benzo ring and its fused indole ring (Fig. 1). The aromatic skeleton is essentially planar.

In the crystal packing, π-π stacking interaction and C—H···π interaction help establish the molecular packing. The shortest centroid-centroid separation is 3.4652 (10) Å, which occurs between the pyrrole parts of the molecules.

Experimental

The compound was obtained according to the method of Du and his coworkers (2008). Colourless block of (I) was grown by slow evaporation of its ethanolic solution.

Refinement

All H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å)and refined as riding with U_{iso}(H) = 1.2U_{eq}(CH) or 1.5U_{eq}(CH_3).

Figures

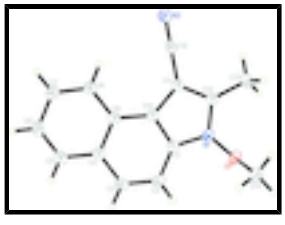

Fig. 1. The molecular structure of (I) showing displacement ellipsoids drawn at the 50% probability level.

1-Methoxy-2-methyl-1*H*-benzo[*f*]indole-3-carbonitrile

Crystal data

$C_{15}H_{12}N_2O$	F(000) = 992
M_r = 236.27	D_x = 1.337 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3553 reflections
a = 18.663 (4) Å	θ = 2.2–27.9°
b = 7.3763 (15) Å	μ = 0.09 mm^{-1}
c = 18.589 (4) Å	*T* = 113 K
β = 113.46 (3)°	Block, colourless

V = 2347.6 (8) Å^3
Z = 8

0.20 × 0.18 × 0.16 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
confocal
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.983, T_{max} = 0.986
11412 measured reflections

2060 independent reflections
1858 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −22→22
k = −8→8
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.04
2060 reflections
166 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
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 1.1054P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0212 (18)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.43321 (5)	0.84231 (12)	0.08385 (5)	0.0257 (3)

N1	0.35813 (6)	0.90176 (14)	0.06827 (6)	0.0203 (3)
N2	0.11930 (6)	1.14000 (15)	−0.10753 (6)	0.0269 (3)
C1	0.32134 (7)	0.87498 (16)	0.11865 (7)	0.0194 (3)
C2	0.34992 (7)	0.79261 (17)	0.19296 (7)	0.0223 (3)
H2	0.4010	0.7503	0.2163	0.027*
C3	0.29960 (7)	0.77742 (16)	0.22936 (7)	0.0223 (3)
H3	0.3171	0.7248	0.2789	0.027*
C4	0.22060 (7)	0.83997 (16)	0.19371 (7)	0.0201 (3)
C5	0.16852 (7)	0.81573 (17)	0.23131 (7)	0.0235 (3)
H5	0.1861	0.7589	0.2800	0.028*
C6	0.09292 (7)	0.87424 (18)	0.19742 (7)	0.0256 (3)
H6	0.0597	0.8579	0.2232	0.031*
C7	0.06515 (8)	0.95940 (18)	0.12338 (7)	0.0249 (3)
H7	0.0138	1.0002	0.1008	0.030*
C8	0.11331 (7)	0.98234 (16)	0.08458 (7)	0.0208 (3)
H8	0.0941	1.0372	0.0355	0.025*
C9	0.19198 (7)	0.92382 (15)	0.11816 (7)	0.0181 (3)
C10	0.24518 (7)	0.93956 (15)	0.08037 (7)	0.0181 (3)
C11	0.23885 (7)	1.00368 (15)	0.00486 (7)	0.0185 (3)
C12	0.31010 (7)	0.97803 (16)	−0.00040 (7)	0.0195 (3)
C13	0.33588 (8)	1.02295 (18)	−0.06433 (7)	0.0253 (3)
H13A	0.3631	1.1367	−0.0531	0.038*
H13B	0.2911	1.0317	−0.1131	0.038*
H13C	0.3700	0.9295	−0.0681	0.038*
C14	0.48901 (8)	0.9831 (2)	0.12264 (9)	0.0327 (4)
H14A	0.4818	1.0829	0.0873	0.049*
H14B	0.5410	0.9362	0.1383	0.049*
H14C	0.4813	1.0239	0.1681	0.049*
C15	0.17262 (7)	1.07923 (16)	−0.05700 (7)	0.0196 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0194 (5)	0.0244 (5)	0.0344 (5)	0.0039 (4)	0.0119 (4)	−0.0008 (4)
N1	0.0163 (5)	0.0211 (5)	0.0235 (6)	0.0016 (4)	0.0079 (4)	−0.0004 (4)
N2	0.0258 (6)	0.0317 (7)	0.0227 (6)	0.0015 (5)	0.0093 (5)	0.0016 (5)
C1	0.0211 (6)	0.0161 (6)	0.0216 (6)	−0.0016 (5)	0.0090 (5)	−0.0021 (5)
C2	0.0203 (6)	0.0193 (6)	0.0237 (7)	0.0015 (5)	0.0049 (5)	−0.0005 (5)
C3	0.0274 (7)	0.0180 (6)	0.0190 (6)	−0.0013 (5)	0.0067 (5)	0.0008 (5)
C4	0.0241 (7)	0.0155 (6)	0.0201 (6)	−0.0031 (5)	0.0082 (5)	−0.0034 (5)
C5	0.0300 (7)	0.0205 (6)	0.0200 (6)	−0.0063 (5)	0.0100 (5)	−0.0031 (5)
C6	0.0265 (7)	0.0283 (7)	0.0258 (7)	−0.0094 (6)	0.0145 (6)	−0.0062 (5)
C7	0.0199 (6)	0.0273 (7)	0.0259 (7)	−0.0043 (5)	0.0076 (5)	−0.0063 (5)
C8	0.0209 (6)	0.0200 (6)	0.0190 (6)	−0.0034 (5)	0.0054 (5)	−0.0030 (5)
C9	0.0203 (6)	0.0142 (6)	0.0187 (6)	−0.0042 (5)	0.0067 (5)	−0.0044 (5)
C10	0.0208 (6)	0.0135 (6)	0.0188 (6)	−0.0030 (5)	0.0065 (5)	−0.0033 (5)
C11	0.0203 (6)	0.0158 (6)	0.0181 (6)	−0.0023 (5)	0.0064 (5)	−0.0019 (4)
C12	0.0227 (7)	0.0153 (6)	0.0198 (6)	−0.0026 (5)	0.0076 (5)	−0.0032 (5)

C13	0.0295 (7)	0.0232 (7)	0.0262 (7)	−0.0014 (5)	0.0143 (6)	−0.0012 (5)
C14	0.0183 (7)	0.0371 (8)	0.0394 (8)	−0.0031 (6)	0.0079 (6)	−0.0001 (6)
C15	0.0225 (7)	0.0191 (6)	0.0192 (6)	−0.0034 (5)	0.0104 (5)	−0.0025 (5)

Geometric parameters (Å, °)

O1—N1	1.3844 (13)	C6—H6	0.9300
O1—C14	1.4442 (16)	C7—C8	1.3685 (18)
N1—C12	1.3559 (16)	C7—H7	0.9300
N1—C1	1.3784 (16)	C8—C9	1.4149 (18)
N2—C15	1.1529 (16)	C8—H8	0.9300
C1—C10	1.3958 (17)	C9—C10	1.4312 (17)
C1—C2	1.4054 (17)	C10—C11	1.4408 (16)
C2—C3	1.3631 (19)	C11—C12	1.3846 (18)
C2—H2	0.9300	C11—C15	1.4245 (18)
C3—C4	1.4311 (18)	C12—C13	1.4862 (17)
C3—H3	0.9300	C13—H13A	0.9600
C4—C5	1.4163 (18)	C13—H13B	0.9600
C4—C9	1.4292 (17)	C13—H13C	0.9600
C5—C6	1.3662 (19)	C14—H14A	0.9600
C5—H5	0.9300	C14—H14B	0.9600
C6—C7	1.4106 (19)	C14—H14C	0.9600
N1—O1—C14	110.19 (9)	C9—C8—H8	119.5
C12—N1—C1	112.19 (10)	C8—C9—C4	118.80 (11)
C12—N1—O1	124.28 (10)	C8—C9—C10	124.02 (11)
C1—N1—O1	123.30 (10)	C4—C9—C10	117.16 (11)
N1—C1—C10	106.64 (11)	C1—C10—C9	119.12 (11)
N1—C1—C2	129.27 (11)	C1—C10—C11	106.30 (11)
C10—C1—C2	124.03 (12)	C9—C10—C11	134.51 (11)
C3—C2—C1	117.16 (11)	C12—C11—C15	123.07 (11)
C3—C2—H2	121.4	C12—C11—C10	108.38 (11)
C1—C2—H2	121.4	C15—C11—C10	128.54 (11)
C2—C3—C4	122.01 (12)	N1—C12—C11	106.49 (11)
C2—C3—H3	119.0	N1—C12—C13	122.83 (11)
C4—C3—H3	119.0	C11—C12—C13	130.67 (12)
C5—C4—C9	118.56 (11)	C12—C13—H13A	109.5
C5—C4—C3	120.91 (11)	C12—C13—H13B	109.5
C9—C4—C3	120.51 (11)	H13A—C13—H13B	109.5
C6—C5—C4	121.21 (12)	C12—C13—H13C	109.5
C6—C5—H5	119.4	H13A—C13—H13C	109.5
C4—C5—H5	119.4	H13B—C13—H13C	109.5
C5—C6—C7	120.10 (12)	O1—C14—H14A	109.5
C5—C6—H6	120.0	O1—C14—H14B	109.5
C7—C6—H6	120.0	H14A—C14—H14B	109.5
C8—C7—C6	120.40 (12)	O1—C14—H14C	109.5
C8—C7—H7	119.8	H14A—C14—H14C	109.5
C6—C7—H7	119.8	H14B—C14—H14C	109.5
C7—C8—C9	120.91 (12)	N2—C15—C11	179.39 (13)
C7—C8—H8	119.5		

C14—O1—N1—C12	93.87 (13)	N1—C1—C10—C9	178.00 (10)
C14—O1—N1—C1	−92.15 (13)	C2—C1—C10—C9	0.53 (18)
C12—N1—C1—C10	−0.59 (13)	N1—C1—C10—C11	0.58 (12)
O1—N1—C1—C10	−175.22 (10)	C2—C1—C10—C11	−176.89 (11)
C12—N1—C1—C2	176.70 (12)	C8—C9—C10—C1	−179.17 (11)
O1—N1—C1—C2	2.08 (19)	C4—C9—C10—C1	−0.57 (16)
N1—C1—C2—C3	−177.49 (11)	C8—C9—C10—C11	−2.7 (2)
C10—C1—C2—C3	−0.62 (18)	C4—C9—C10—C11	175.95 (12)
C1—C2—C3—C4	0.78 (18)	C1—C10—C11—C12	−0.40 (13)
C2—C3—C4—C5	177.32 (11)	C9—C10—C11—C12	−177.24 (12)
C2—C3—C4—C9	−0.89 (18)	C1—C10—C11—C15	178.68 (11)
C9—C4—C5—C6	−1.41 (18)	C9—C10—C11—C15	1.8 (2)
C3—C4—C5—C6	−179.65 (11)	C1—N1—C12—C11	0.33 (13)
C4—C5—C6—C7	0.48 (19)	O1—N1—C12—C11	174.90 (10)
C5—C6—C7—C8	0.70 (19)	C1—N1—C12—C13	179.24 (11)
C6—C7—C8—C9	−0.91 (18)	O1—N1—C12—C13	−6.20 (18)
C7—C8—C9—C4	−0.04 (17)	C15—C11—C12—N1	−179.09 (10)
C7—C8—C9—C10	178.54 (11)	C10—C11—C12—N1	0.05 (13)
C5—C4—C9—C8	1.18 (17)	C15—C11—C12—C13	2.1 (2)
C3—C4—C9—C8	179.42 (10)	C10—C11—C12—C13	−178.73 (12)
C5—C4—C9—C10	−177.50 (10)	C12—C11—C15—N2	20 (14)
C3—C4—C9—C10	0.75 (17)	C10—C11—C15—N2	−159 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cg3^{i}	0.93	2.65	3.3956 (15)	138

Symmetry codes: (i) *x*, −*y*−1, *z*−1/2.

Fig. 1