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(*E*)-Methyl 3-(1*H*-indol-3-yl)acrylate

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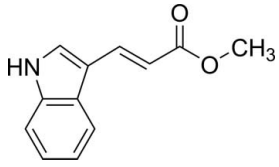
Key indicators: single-crystal X-ray study; T = 288 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.136; data-to-parameter ratio = 16.9.

In the title compound, $C_{12}H_{11}NO_2$, the indole and methyl acrylate mean planes are inclined at an angle of 10.6 (1)°. In the crystal, N—H$\cdots\pi$ interactions link molecules into chains along [010] and weak intermolecular C—H$\cdots$O hydrogen bonds further consolidate the crystal packing.

Related literature

For general background to the synthesis of 3-substituted indole derivatives as precursors of potent anti-inflammatory and analgesic agents, see Radwan *et al.* (1997). For details of the synthesis, see García-Rubia *et al.* (2010). For related structures, see: Bhella *et al.* (2009); Hou & Li (2011).



Experimental

Crystal data

$C_{12}H_{11}NO_2$
M_r = 201.22
Monoclinic, $P2_1/c$
a = 5.884 (3) Å
b = 7.923 (5) Å
c = 21.898 (13) Å
β = 93.54 (3)°
V = 1018.9 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 288 K
0.43 × 0.26 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.963, T_{max} = 0.980
9616 measured reflections
2333 independent reflections
1730 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.136
S = 1.08
2333 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

Cg is the centroid of the C1–C6 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$\cdots$O1^{i}	0.93	2.65	3.558 (2)	165
C12—H12$B\cdots$O1^{ii}	0.96	2.63	3.540 (3)	159
N1—H1$A\cdots Cg^{iii}$	0.86	2.52	3.189 (3)	135

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5189).

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supporting information

Acta Cryst. (2011). E**67**, o3290 [https://doi.org/10.1107/S1600536811046745]

(*E*)-Methyl 3-(1*H*-indol-3-yl)acrylate

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S1. Comment

Indole skeleton is a key component of many biologically active compounds. Radwan *et al.* (1997) have synthesized and evaluated of 3-substituted indole derivatives as precursors of potent anti-inflammatory and analgesic agents. Recently, Bhella *et al.* (2009) reported a series of compounds with the similar structures. In this paper, we report the crystal structure of the title compound.

In the tiltle compound (Fig. 1), all bond lengths and angles are normal and comparable with those reported for close structures (Bhella *et al.*, 2009; Hou & Li, 2011). The dihedral angle between the indole and methyl acrylate mean planes is 10.6 (1)°. In the crystal structure, N—H···π interactions (Table 1) link molecules into chians along [010], and weak intermolecular C—H···O hydrogen bonds (Table 1) consolidate further the crystal packing.

S2. Experimental

The title compound was prepared according to the literature (García-Rubia *et al.*, 2010). Single crystals suitable for X-ray diffraction were prepared by slow evaporation a mixture of dichloromethane and petroleum (60–90 °C) at room temperature.

S3. Refinement

C-bound H atoms were placed in calculated positions (C—H 0.93 and 0.96 Å) and were included in the refinement in the riding model with U_{iso}(H) = 1.2 and 1.5 U_{eq}(C). The N-bound H atom was placed in calculated position with N—H = 0.86 Å and refined with U_{iso}(H) = 1.2 U_{eq}(N).

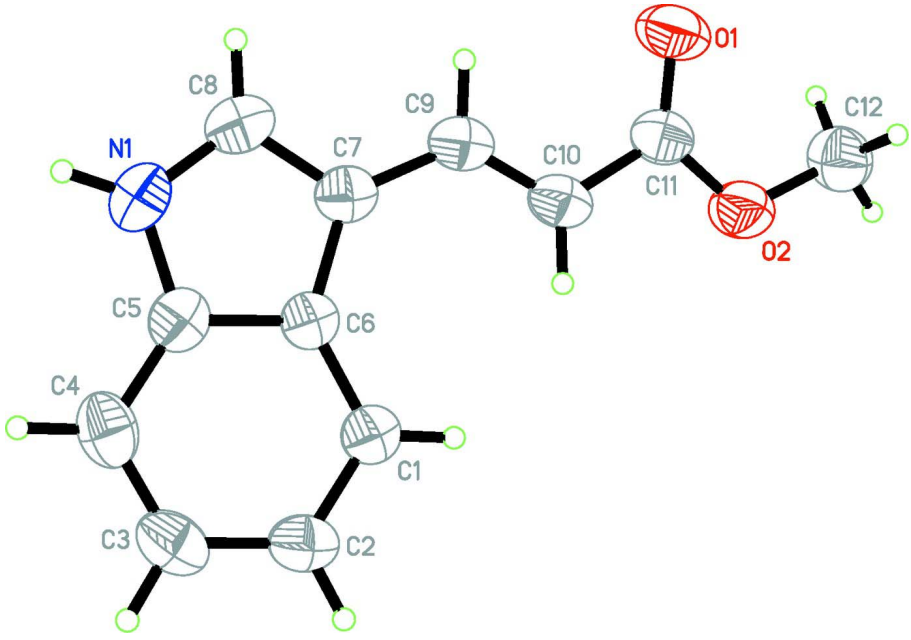

Figure 1

The molecular structure of the title compound showing the atomic numbering and 50% probability displacemnet ellipsoids.

(*E*)-Methyl 3-(1*H*-indol-3-yl)acrylate

Crystal data

$C_{12}H_{11}NO_2$
$M_r = 201.22$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.884$ (3) Å
$b = 7.923$ (5) Å
$c = 21.898$ (13) Å
$\beta = 93.54$ (3)°
$V = 1018.9$ (10) Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.312$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6974 reflections
$\theta = 3.2$–27.5°
$\mu = 0.09$ mm^{-1}
$T = 288$ K
Block, colourless
0.43 × 0.26 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.963$, $T_{max} = 0.980$
9616 measured reflections
2333 independent reflections
1730 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -6 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.136$
$S = 1.08$
2333 reflections
138 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
$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 0.0624P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.026 (5)

Special details

Experimental. (See detailed section in the paper)

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}
C1	0.9472 (2)	0.64568 (18)	0.23712 (6)	0.0434 (3)
H1	1.0528	0.7010	0.2143	0.052*
C2	0.9795 (3)	0.63514 (19)	0.30016 (7)	0.0502 (4)
H2	1.1092	0.6829	0.3195	0.060*
C3	0.8210 (3)	0.55410 (19)	0.33566 (7)	0.0534 (4)
H3	0.8461	0.5510	0.3780	0.064*
C4	0.6291 (3)	0.47926 (19)	0.30863 (7)	0.0524 (4)
H4	0.5245	0.4244	0.3319	0.063*
C5	0.5973 (2)	0.48890 (17)	0.24505 (7)	0.0434 (3)
C6	0.7520 (2)	0.57135 (16)	0.20809 (6)	0.0379 (3)
C7	0.6584 (2)	0.55697 (17)	0.14540 (6)	0.0428 (3)
C8	0.4580 (2)	0.46741 (19)	0.14818 (7)	0.0503 (4)
H8	0.3616	0.4387	0.1145	0.060*
C9	0.7440 (3)	0.61468 (18)	0.08871 (7)	0.0461 (4)
H9	0.6473	0.6000	0.0539	0.055*
C10	0.9444 (3)	0.68641 (19)	0.07991 (6)	0.0474 (4)
H10	1.0461	0.7067	0.1133	0.057*
C11	1.0071 (3)	0.73389 (19)	0.01826 (6)	0.0462 (4)
C12	1.3035 (3)	0.8419 (3)	−0.03879 (8)	0.0621 (5)
H12A	1.2504	0.7638	−0.0700	0.093*
H12B	1.4669	0.8430	−0.0359	0.093*
H12C	1.2477	0.9528	−0.0490	0.093*

N1	0.4222 (2)	0.42746 (16)	0.20675 (6)	0.0520 (4)
H1A	0.3071	0.3719	0.2184	0.062*
O1	0.8851 (2)	0.72446 (18)	−0.02800 (5)	0.0711 (4)
O2	1.22147 (19)	0.79075 (16)	0.01910 (5)	0.0607 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0429 (7)	0.0419 (7)	0.0452 (8)	0.0007 (6)	0.0015 (6)	−0.0008 (6)
C2	0.0524 (8)	0.0507 (8)	0.0463 (8)	0.0032 (7)	−0.0077 (7)	−0.0025 (6)
C3	0.0702 (10)	0.0491 (8)	0.0404 (7)	0.0101 (7)	−0.0006 (7)	0.0023 (6)
C4	0.0644 (10)	0.0426 (7)	0.0517 (8)	0.0047 (7)	0.0149 (7)	0.0057 (6)
C5	0.0441 (7)	0.0340 (7)	0.0521 (8)	0.0027 (6)	0.0037 (6)	−0.0018 (6)
C6	0.0396 (7)	0.0316 (6)	0.0426 (7)	0.0043 (5)	0.0018 (6)	−0.0013 (5)
C7	0.0439 (7)	0.0387 (7)	0.0452 (7)	0.0032 (6)	−0.0012 (6)	−0.0043 (6)
C8	0.0449 (8)	0.0497 (8)	0.0553 (9)	−0.0006 (6)	−0.0049 (7)	−0.0077 (7)
C9	0.0496 (8)	0.0454 (8)	0.0423 (7)	0.0048 (6)	−0.0055 (6)	−0.0036 (6)
C10	0.0535 (8)	0.0499 (8)	0.0379 (7)	0.0033 (7)	−0.0037 (6)	−0.0035 (6)
C11	0.0471 (8)	0.0499 (8)	0.0412 (7)	0.0063 (6)	0.0001 (6)	−0.0032 (6)
C12	0.0568 (9)	0.0772 (11)	0.0535 (9)	0.0000 (9)	0.0116 (8)	0.0016 (8)
N1	0.0453 (7)	0.0484 (7)	0.0625 (8)	−0.0086 (5)	0.0057 (6)	−0.0025 (6)
O1	0.0614 (8)	0.1069 (10)	0.0435 (6)	−0.0047 (7)	−0.0078 (5)	0.0081 (6)
O2	0.0550 (7)	0.0826 (8)	0.0444 (6)	−0.0088 (6)	0.0013 (5)	−0.0001 (5)

Geometric parameters (Å, º)

C1—C2	1.384 (2)	C8—N1	1.350 (2)
C1—C6	1.407 (2)	C8—H8	0.9300
C1—H1	0.9300	C9—C10	1.334 (2)
C2—C3	1.406 (2)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.470 (2)
C3—C4	1.376 (2)	C10—H10	0.9300
C3—H3	0.9300	C11—O1	1.2075 (18)
C4—C5	1.396 (2)	C11—O2	1.338 (2)
C4—H4	0.9300	C12—O2	1.442 (2)
C5—N1	1.377 (2)	C12—H12A	0.9600
C5—C6	1.415 (2)	C12—H12B	0.9600
C6—C7	1.452 (2)	C12—H12C	0.9600
C7—C8	1.380 (2)	N1—H1A	0.8600
C7—C9	1.443 (2)		
C2—C1—C6	118.88 (14)	N1—C8—H8	124.9
C2—C1—H1	120.6	C7—C8—H8	124.9
C6—C1—H1	120.6	C10—C9—C7	128.21 (14)
C1—C2—C3	121.62 (14)	C10—C9—H9	115.9
C1—C2—H2	119.2	C7—C9—H9	115.9
C3—C2—H2	119.2	C9—C10—C11	121.07 (13)
C4—C3—C2	120.92 (15)	C9—C10—H10	119.5

C4—C3—H3	119.5	C11—C10—H10	119.5
C2—C3—H3	119.5	O1—C11—O2	122.92 (15)
C3—C4—C5	117.46 (15)	O1—C11—C10	125.77 (16)
C3—C4—H4	121.3	O2—C11—C10	111.31 (12)
C5—C4—H4	121.3	O2—C12—H12A	109.5
N1—C5—C4	129.60 (14)	O2—C12—H12B	109.5
N1—C5—C6	107.38 (14)	H12A—C12—H12B	109.5
C4—C5—C6	123.02 (14)	O2—C12—H12C	109.5
C1—C6—C5	118.10 (13)	H12A—C12—H12C	109.5
C1—C6—C7	135.37 (13)	H12B—C12—H12C	109.5
C5—C6—C7	106.53 (12)	C8—N1—C5	109.94 (13)
C8—C7—C9	123.06 (13)	C8—N1—H1A	125.0
C8—C7—C6	105.90 (13)	C5—N1—H1A	125.0
C9—C7—C6	131.02 (13)	C11—O2—C12	116.66 (12)
N1—C8—C7	110.25 (13)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.65	3.558 (2)	165
C12—H12*B*···O1^{ii}	0.96	2.63	3.540 (3)	159
N1—H1*A*···*Cg*^{iii}	0.86	2.52	3.189 (3)	135

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