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(E)-Methyl 3-(1H-indol-2-yl)acrylate

Rui-Bin Hou and Dong-Feng Li*

 School of Chemistry and Life Sciences, Changchun University of Technology,
 Changchun 130012, People's Republic of China

Correspondence e-mail: lidongfeng@mail.ccut.edu.cn

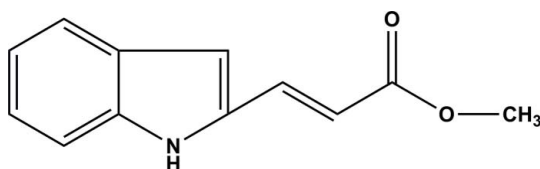
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.049; wR factor = 0.133; data-to-parameter ratio = 17.0.

The title compound, $\text{C}_{12}\text{H}_{11}\text{NO}_2$, is close to being planar (r.m.s. deviation for the non-H atoms = 0.033 Å). In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, generating $C(7)$ chains running along the b axis. A weak $\text{C}-\text{H}\cdots\text{O}$ interaction helps to establish the packing.

Related literature

For background literature related to indoles in medicinal chemistry, see: Zeynep *et al.* (2005). For details of the synthesis, see García-Rubia *et al.* (2010).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_{11}\text{NO}_2$
 $M_r = 201.22$
 Orthorhombic, $Pbca$
 $a = 7.735$ (5) Å

 $b = 11.324$ (5) Å
 $c = 23.236$ (10) Å
 $V = 2035.4$ (17) Å³
 $Z = 8$

 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 296$ K
 $0.39 \times 0.27 \times 0.22$ mm

Data collection

 Rigaku R-Axis RAPID
 diffractometer
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.966$, $T_{\max} = 0.980$

 18445 measured reflections
 2326 independent reflections
 1555 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.065$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.133$
 $S = 1.04$
 2326 reflections
 137 parameters

 1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.98	1.93	2.900 (2)	174
$\text{C5}-\text{H5}\cdots\text{O2}^{ii}$	0.93	2.57	3.390 (3)	147

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 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: HB5951).

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supporting information

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(E)-Methyl 3-(1*H*-indol-2-yl)acrylate**Rui-Bin Hou and Dong-Feng Li****S1. Comment**

Indole derivatives constitute an important class of therapeutic agents in medicinal chemistry including anticancer, antioxidant, antirheumatoidal and anti-HIVv (e.g. Zeynep *et al.*, 2005). We recently synthesized some indole derivatives as histone deacetylase (HDAC) inhibitors with the precursor. In this paper, we report the crystal structure of the title compound, (I).

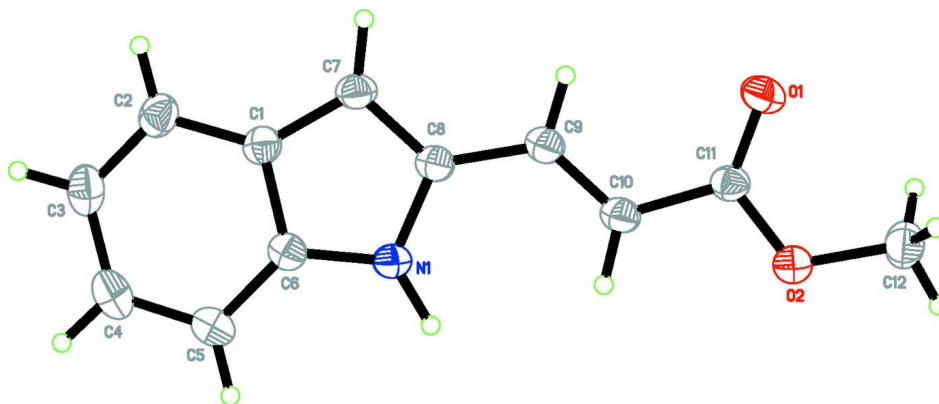
The molecular structure of title compound, C₁₂H₁₃O₂N, as shown in Fig. 1, all bond lengths and angles are in the normal ranges. All non-hydrogen atoms are nearly coplanar. In the crystal, the intermolecular N—H···O hydrogen bonds link the molecules into chains along b direction.

S2. Experimental

The title compound was prepared according to the literature method (García-Rubia *et al.*, 2010). Colourless blocks of (I) were prepared by slow evaporation of a solution in a mixture of dichloromethane and petroleum (60–90 °C) at room temperature.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 and 0.97 Å) and were included in the refinement in the riding model with $U_{\text{iso}}(\text{H}) = 1.5$ or $1.2 U_{\text{eq}}(\text{C})$. The N-bound H atom was located from a difference map and refined with the distance restraints N—H = 0.90 Å and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{N})$.

**Figure 1**

The title compound, with displacement ellipsoids of non-H atoms drawn at the 30% probability level.

(E)-Methyl 3-(1*H*-indol-2-yl)prop-2-enoate*Crystal data*

$C_{12}H_{11}NO_2$	$F(000) = 848$
$M_r = 201.22$	$D_x = 1.313 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ac 2ab	Cell parameters from 10451 reflections
$a = 7.735 (5) \text{ \AA}$	$\theta = 3.2\text{--}27.5^\circ$
$b = 11.324 (5) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 23.236 (10) \text{ \AA}$	$T = 296 \text{ K}$
$V = 2035.4 (17) \text{ \AA}^3$	Block, colorless
$Z = 8$	$0.39 \times 0.27 \times 0.22 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	18445 measured reflections
Radiation source: fine-focus sealed tube	2326 independent reflections
Graphite monochromator	1555 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.065$
Absorption correction: multi-scan (<i>ABSCOR</i> ; Higashi, 1995)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.2^\circ$
$T_{\text{min}} = 0.966$, $T_{\text{max}} = 0.980$	$h = -10 \rightarrow 10$
	$k = -14 \rightarrow 13$
	$l = -30 \rightarrow 29$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.2072P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
2326 reflections	$(\Delta/\sigma)_{\text{max}} = 0.003$
137 parameters	$\Delta\rho_{\text{max}} = 0.14 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5285 (2)	0.89360 (14)	0.82265 (7)	0.0413 (4)
C2	0.6101 (3)	0.86472 (16)	0.77057 (7)	0.0505 (5)
H2	0.6292	0.9224	0.7428	0.061*
C3	0.6611 (3)	0.75051 (17)	0.76123 (8)	0.0571 (5)

H3	0.7158	0.7310	0.7269	0.068*
C4	0.6323 (3)	0.66264 (17)	0.80249 (9)	0.0592 (6)
H4	0.6662	0.5855	0.7946	0.071*
C5	0.5548 (3)	0.68769 (16)	0.85450 (8)	0.0511 (5)
H5	0.5374	0.6293	0.8821	0.061*
C6	0.5037 (2)	0.80400 (14)	0.86409 (7)	0.0399 (4)
C7	0.4614 (2)	0.99847 (15)	0.84673 (7)	0.0448 (4)
H7	0.4585	1.0721	0.8290	0.054*
C8	0.4012 (2)	0.97292 (14)	0.90079 (7)	0.0401 (4)
C9	0.3182 (2)	1.05130 (14)	0.94093 (7)	0.0421 (4)
H9	0.3052	1.1292	0.9290	0.051*
C10	0.2580 (2)	1.02608 (14)	0.99292 (7)	0.0422 (4)
H10	0.2693	0.9498	1.0072	0.051*
C11	0.1744 (2)	1.11639 (13)	1.02804 (7)	0.0397 (4)
C12	0.0416 (3)	1.15364 (17)	1.11785 (8)	0.0573 (5)
H12A	0.1057	1.2260	1.1206	0.086*
H12B	0.0332	1.1180	1.1552	0.086*
H12C	-0.0723	1.1699	1.1035	0.086*
N1	0.4262 (2)	0.85400 (11)	0.91135 (6)	0.0409 (4)
H1	0.3997	0.8130	0.9473	0.061*
O1	0.1477 (2)	1.21728 (10)	1.01398 (5)	0.0635 (4)
O2	0.12888 (17)	1.07412 (10)	1.07924 (5)	0.0484 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0440 (11)	0.0430 (9)	0.0370 (8)	-0.0047 (7)	-0.0065 (7)	-0.0006 (7)
C2	0.0554 (13)	0.0565 (11)	0.0394 (9)	-0.0110 (9)	-0.0013 (8)	-0.0037 (8)
C3	0.0526 (13)	0.0653 (12)	0.0533 (11)	-0.0077 (10)	0.0060 (9)	-0.0191 (9)
C4	0.0546 (14)	0.0508 (11)	0.0724 (13)	0.0036 (9)	-0.0002 (10)	-0.0176 (10)
C5	0.0531 (12)	0.0391 (9)	0.0609 (11)	-0.0005 (8)	-0.0035 (9)	0.0007 (8)
C6	0.0383 (10)	0.0387 (8)	0.0428 (9)	-0.0013 (7)	-0.0046 (7)	-0.0006 (7)
C7	0.0548 (12)	0.0391 (8)	0.0405 (9)	-0.0009 (8)	-0.0044 (8)	0.0066 (7)
C8	0.0431 (10)	0.0365 (8)	0.0406 (9)	-0.0011 (7)	-0.0039 (7)	0.0014 (7)
C9	0.0462 (11)	0.0359 (8)	0.0443 (9)	0.0017 (7)	-0.0035 (8)	0.0016 (7)
C10	0.0475 (11)	0.0351 (8)	0.0440 (9)	0.0019 (7)	-0.0035 (8)	0.0037 (7)
C11	0.0442 (10)	0.0370 (9)	0.0377 (8)	-0.0009 (7)	-0.0048 (7)	0.0025 (7)
C12	0.0559 (13)	0.0626 (12)	0.0533 (11)	0.0067 (10)	0.0079 (9)	-0.0038 (9)
N1	0.0468 (9)	0.0362 (7)	0.0396 (7)	0.0000 (6)	0.0003 (6)	0.0048 (6)
O1	0.0983 (12)	0.0409 (7)	0.0514 (8)	0.0168 (7)	0.0050 (7)	0.0073 (6)
O2	0.0572 (9)	0.0428 (6)	0.0452 (7)	0.0047 (6)	0.0062 (6)	0.0043 (5)

Geometric parameters (Å, °)

C1—C2	1.403 (2)	C8—N1	1.383 (2)
C1—C7	1.412 (2)	C8—C9	1.439 (2)
C1—C6	1.412 (2)	C9—C10	1.326 (2)
C2—C3	1.370 (3)	C9—H9	0.9300

C2—H2	0.9300	C10—C11	1.460 (2)
C3—C4	1.400 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—O1	1.2060 (19)
C4—C5	1.378 (3)	C11—O2	1.330 (2)
C4—H4	0.9300	C12—O2	1.439 (2)
C5—C6	1.393 (2)	C12—H12A	0.9600
C5—H5	0.9300	C12—H12B	0.9600
C6—N1	1.373 (2)	C12—H12C	0.9600
C7—C8	1.371 (2)	N1—H1	0.9772
C7—H7	0.9300		
C2—C1—C7	134.69 (16)	C7—C8—C9	127.99 (15)
C2—C1—C6	118.79 (16)	N1—C8—C9	123.26 (15)
C7—C1—C6	106.51 (15)	C10—C9—C8	127.91 (16)
C3—C2—C1	119.11 (17)	C10—C9—H9	116.0
C3—C2—H2	120.4	C8—C9—H9	116.0
C1—C2—H2	120.4	C9—C10—C11	120.93 (15)
C2—C3—C4	121.12 (18)	C9—C10—H10	119.5
C2—C3—H3	119.4	C11—C10—H10	119.5
C4—C3—H3	119.4	O1—C11—O2	122.54 (15)
C5—C4—C3	121.56 (17)	O1—C11—C10	126.04 (15)
C5—C4—H4	119.2	O2—C11—C10	111.42 (13)
C3—C4—H4	119.2	O2—C12—H12A	109.5
C4—C5—C6	117.27 (17)	O2—C12—H12B	109.5
C4—C5—H5	121.4	H12A—C12—H12B	109.5
C6—C5—H5	121.4	O2—C12—H12C	109.5
N1—C6—C5	129.91 (16)	H12A—C12—H12C	109.5
N1—C6—C1	107.97 (14)	H12B—C12—H12C	109.5
C5—C6—C1	122.13 (16)	C6—N1—C8	108.71 (13)
C8—C7—C1	108.11 (15)	C6—N1—H1	125.4
C8—C7—H7	125.9	C8—N1—H1	125.8
C1—C7—H7	125.9	C11—O2—C12	117.17 (13)
C7—C8—N1	108.70 (15)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O1 ⁱ	0.98	1.93	2.900 (2)	174
C5—H5 \cdots O2 ⁱⁱ	0.93	2.57	3.390 (3)	147

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