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# (*E*)-Methyl 3-(1*H*-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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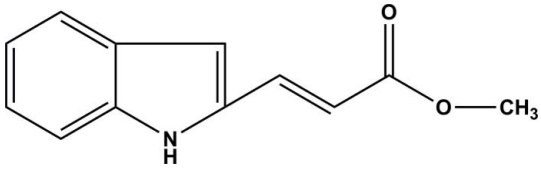
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.049; $wR$ factor = 0.133; data-to-parameter ratio = 17.0.

The title compound, $C_{12}H_{11}NO_2$, is close to being planar (r.m.s. deviation for the non-H atoms = 0.033 Å). In the crystal, molecules are linked by N—H···O hydrogen bonds, generating $C(7)$ chains running along the $b$ axis. A weak C—H···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

$C_{12}H_{11}NO_2$
$M_r$ = 201.22
Orthorhombic, *Pbca*
$a$ = 7.735 (5) Å
$b$ = 11.324 (5) Å
$c$ = 23.236 (10) Å
$V$ = 2035.4 (17) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.39 × 0.27 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.98 | 1.93 | 2.900 (2) | 174 |
| C5—H5···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/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: HB5951).

## References

García-Rubia, A., Urones, B., Arrayás, R. G. & Carretero, J. C. (2010). *Chem. Eur. J.* **16**, 9676–9685.
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# supplementary materials

*Acta Cryst.* (2011). E**67**, o2197 [ **doi:10.1107/S1600536811030121** ]

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

**R.-B. Hou and D.-F. Li**

## 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, $C_{12}H_{13}O_2N$, 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.

## 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.

## 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 $U_{iso}$(H) = 1.5 or 1.2 $U_{eq}$(C). The N-bound H atom was located from a difference map and refined with the distance restraints N—H = 0.90 Å and $U_{iso}$(H) = 1.5 $U_{eq}$(N).

## Figures

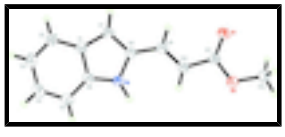

Fig. 1. The title compound, with displacement ellipsoids of non-H atoms drawn at the 30% probalility level.

## (*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 Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 10451 reflections |
| *a* = 7.735 (5) Å | θ = 3.2–27.5° |
| *b* = 11.324 (5) Å | μ = 0.09 mm$^{-1}$ |
| *c* = 23.236 (10) Å | *T* = 296 K |

| | |
|---|---|
| $V$ = 2035.4 (17) Å$^3$ | Block, colorless |
| $Z$ = 8 | 0.39 × 0.27 × 0.22 mm |

*Data collection*

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

*Refinement*

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

*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 | 0.5285 (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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.98 | 1.93 | 2.900 (2) | 174 |
| C5—H5···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.

**Fig. 1**