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# 7-Methyl-1*H*-indole-2,3-dione

Myrria-Tahisha A. Lyncee,[a] Vasumathi Desikan,[a] James A. Golen[b] and David R. Manke[b]*

[a]Department of Science & Math, Massasoit Community College, 1 Massasoit Boulevard, Brockton, MA 02302, USA, and [b]Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, 285 Old Westport Road, North Dartmouth, MA 02747, USA. *Correspondence e-mail: dmanke@umassd.edu

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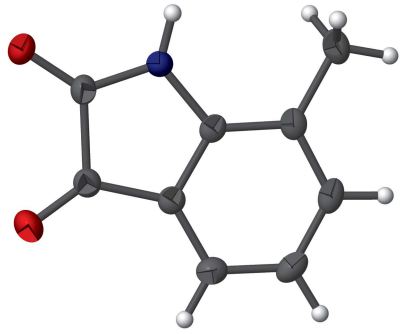
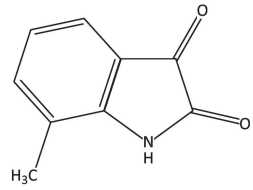
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_9H_7NO_2$, has a single molecule in the asymmetric unit, with the non-H atoms possessing a mean deviation from planarity of 0.034 Å. In the crystal, the molecules dimerize through pairs of N—H···O hydrogen bonds. The nine-membered rings of the isatins stack along the *b* axis, through parallel slipped $\pi$–$\pi$ interactions [intercentroid distance = 3.8832 (4) Å, interplanar distance = 3.4038 (7) Å and slippage = 1.8690 (12) Å].

**3D view**



**Chemical scheme**




## Structure description

As part of our continuing study of the intermolecular interactions of substituted isatins, we report the crystal structure of 7-methyl-1*H*-indole-2,3-dione (Fig. 1). The molecule is nearly planar, with the non-H atoms in the structure demonstrating a mean deviation from planarity of 0.034 Å. The bond lengths and angles are consistent with those observed in the reported *N*-substituted derivative of 7-methyl-1*H*-indole-2,3-dione (Mironova *et al.*, 2015).

In the crystal, the molecules dimerize through pairs of N1—H1···O1$^{i}$ hydrogen bonds (Table 1). This dimerization is observed in other 7-substituted isatin compounds (Garden *et al.*, 2006; Golen & Manke, 2016*a*,*b*; Mohamed *et al.*, 2008). The one reported exception is 7-chloroisatin, which forms a tetrameric assembly though its N—H···O hydrogen bonds (Sun & Cai, 2010). The nine-membered rings of the 7-methylisatin units stack along [010] with parallel slipped $\pi$–$\pi$ interactions [intercentroid distance = 3.8832 (4) Å, interplanar distance = 3.4038 (7) Å and slippage = 1.8690 (12) Å]. The packing of the title compound, including hydrogen bonding, is shown in Fig. 2.

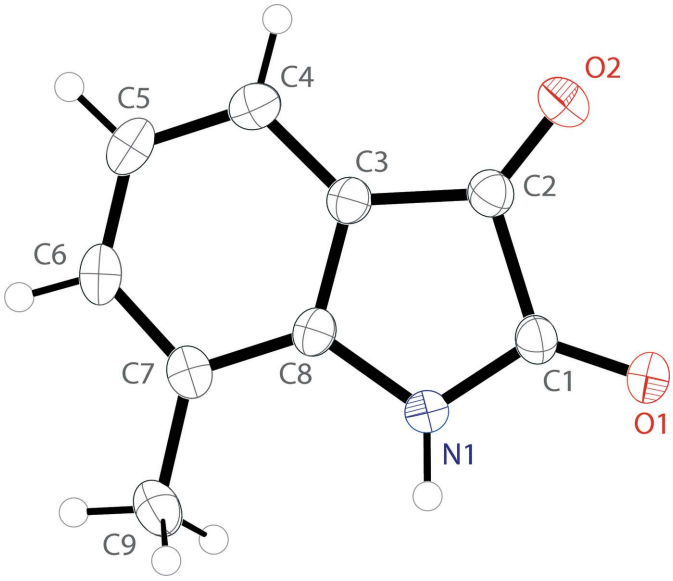



**Figure 1**
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

## Synthesis and crystallization

A commercial sample (AK Scientific) of 7-methylisatin was recrystallized by the slow evaporation of an acetonitrile solution to yield orange plates suitable for single-crystal diffraction analysis.

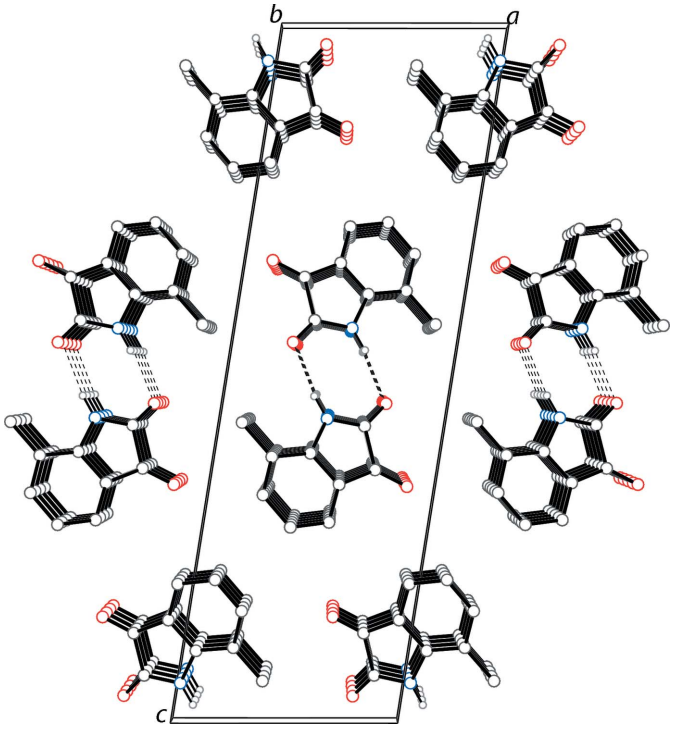



**Figure 2**
The molecular packing of the title compound along the *b* axis, with hydrogen bonds shown as dashed lines.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.88 (1) | 2.03 (1) | 2.8907 (17) | 170 (2) |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_9H_7NO_2$ |
| $M_r$ | 161.16 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 200 |
| *a*, *b*, *c* (Å) | 7.8114 (10), 3.8832 (4), 24.362 (3) |
| $\beta$ (°) | 99.055 (5) |
| *V* (Å$^3$) | 729.76 (15) |
| *Z* | 4 |
| Radiation type | Mo *Kα* |
| $\mu$ (mm$^{-1}$) | 0.11 |
| Crystal size (mm) | 0.19 × 0.18 × 0.04 |
| Data collection | |
| Diffractometer | Bruker D8 Venture CMOS |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) |
| $T_{min}$, $T_{max}$ | 0.701, 0.745 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 18978, 1342, 1147 |
| $R_{int}$ | 0.050 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.605 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.036, 0.089, 1.09 |
| No. of reflections | 1342 |
| No. of parameters | 114 |
| No. of restraints | 1 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.20, −0.17 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Funding information

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# full crystallographic data

*IUCrData* (2017). **2**, x170378 [https://doi.org/10.1107/S2414314617003789]

## 7-Methyl-1*H*-indole-2,3-dione

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### 7-Methyl-1*H*-indole-2,3-dione

*Crystal data*

$C_9H_7NO_2$
$M_r$ = 161.16
Monoclinic, $P2_1/n$
$a$ = 7.8114 (10) Å
$b$ = 3.8832 (4) Å
$c$ = 24.362 (3) Å
$\beta$ = 99.055 (5)°
$V$ = 729.76 (15) Å$^3$
$Z$ = 4
$F(000)$ = 336
$D_x$ = 1.467 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 7064 reflections
$\theta$ = 2.9–25.2°
$\mu$ = 0.11 mm$^{-1}$
$T$ = 200 K
Plate, orange
0.19 × 0.18 × 0.04 mm

*Data collection*

Bruker D8 Venture CMOS diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min}$ = 0.701, $T_{max}$ = 0.745
18978 measured reflections
1342 independent reflections
1147 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 3.4°
$h$ = −9→9
$k$ = −4→4
$l$ = −29→29

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.089
$S$ = 1.09
1342 reflections
114 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.3841P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.035 (5)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.71863 (14) | −0.0390 (3) | 0.54254 (4) | 0.0339 (3) |
| O2 | 0.86187 (14) | 0.1882 (3) | 0.65601 (5) | 0.0368 (3) |
| N1 | 0.47768 (16) | 0.2518 (4) | 0.56258 (5) | 0.0245 (3) |
| H1 | 0.4086 (18) | 0.206 (5) | 0.5316 (5) | 0.029* |
| C1 | 0.64162 (19) | 0.1320 (4) | 0.57297 (6) | 0.0247 (4) |
| C2 | 0.71578 (19) | 0.2489 (4) | 0.63341 (6) | 0.0249 (4) |
| C3 | 0.57186 (19) | 0.4265 (4) | 0.65299 (6) | 0.0227 (4) |
| C4 | 0.5546 (2) | 0.5703 (4) | 0.70413 (6) | 0.0273 (4) |
| H4 | 0.6491 | 0.5730 | 0.7339 | 0.033* |
| C5 | 0.3958 (2) | 0.7094 (4) | 0.71040 (7) | 0.0303 (4) |
| H5 | 0.3804 | 0.8089 | 0.7449 | 0.036* |
| C6 | 0.2585 (2) | 0.7045 (4) | 0.66648 (7) | 0.0286 (4) |
| H6 | 0.1515 | 0.8049 | 0.6719 | 0.034* |
| C7 | 0.27078 (19) | 0.5583 (4) | 0.61465 (6) | 0.0245 (4) |
| C8 | 0.43097 (19) | 0.4204 (4) | 0.60971 (6) | 0.0217 (4) |
| C9 | 0.1214 (2) | 0.5477 (5) | 0.56768 (7) | 0.0332 (4) |
| H9A | 0.0248 | 0.6828 | 0.5776 | 0.050* |
| H9B | 0.0843 | 0.3085 | 0.5606 | 0.050* |
| H9C | 0.1575 | 0.6447 | 0.5342 | 0.050* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0267 (6) | 0.0463 (8) | 0.0293 (6) | 0.0072 (5) | 0.0062 (5) | −0.0098 (5) |
| O2 | 0.0240 (6) | 0.0523 (8) | 0.0326 (6) | 0.0067 (6) | −0.0001 (5) | −0.0013 (6) |
| N1 | 0.0217 (7) | 0.0307 (7) | 0.0208 (7) | 0.0019 (6) | 0.0023 (5) | −0.0027 (6) |
| C1 | 0.0209 (7) | 0.0282 (8) | 0.0258 (8) | 0.0013 (7) | 0.0061 (6) | 0.0003 (7) |
| C2 | 0.0233 (8) | 0.0273 (8) | 0.0243 (8) | 0.0005 (7) | 0.0045 (6) | 0.0022 (6) |
| C3 | 0.0235 (8) | 0.0226 (8) | 0.0226 (8) | −0.0008 (6) | 0.0051 (6) | 0.0013 (6) |
| C4 | 0.0302 (9) | 0.0282 (8) | 0.0233 (8) | −0.0022 (7) | 0.0036 (6) | −0.0007 (7) |
| C5 | 0.0393 (10) | 0.0280 (9) | 0.0263 (8) | 0.0002 (7) | 0.0133 (7) | −0.0033 (7) |
| C6 | 0.0290 (8) | 0.0243 (8) | 0.0356 (9) | 0.0034 (7) | 0.0146 (7) | 0.0013 (7) |
| C7 | 0.0237 (8) | 0.0212 (8) | 0.0294 (8) | 0.0010 (6) | 0.0070 (6) | 0.0047 (6) |
| C8 | 0.0248 (8) | 0.0198 (8) | 0.0218 (7) | −0.0007 (6) | 0.0077 (6) | 0.0025 (6) |
| C9 | 0.0243 (8) | 0.0364 (10) | 0.0389 (10) | 0.0063 (7) | 0.0044 (7) | 0.0018 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.2219 (18) | C4—C5 | 1.383 (2) |
| O2—C2 | 1.2096 (18) | C5—H5 | 0.9500 |
| N1—H1 | 0.875 (9) | C5—C6 | 1.391 (2) |
| N1—C1 | 1.348 (2) | C6—H6 | 0.9500 |
| N1—C8 | 1.4184 (19) | C6—C7 | 1.401 (2) |
| C1—C2 | 1.562 (2) | C7—C8 | 1.384 (2) |
| C2—C3 | 1.461 (2) | C7—C9 | 1.501 (2) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.391 (2) | C9—H9A | 0.9800 |
| C3—C8 | 1.399 (2) | C9—H9B | 0.9800 |
| C4—H4 | 0.9500 | C9—H9C | 0.9800 |
| | | | |
| C1—N1—H1 | 122.1 (11) | C6—C5—H5 | 119.8 |
| C1—N1—C8 | 111.40 (12) | C5—C6—H6 | 118.5 |
| C8—N1—H1 | 126.2 (11) | C5—C6—C7 | 123.01 (15) |
| O1—C1—N1 | 128.12 (14) | C7—C6—H6 | 118.5 |
| O1—C1—C2 | 125.78 (13) | C6—C7—C9 | 122.86 (14) |
| N1—C1—C2 | 106.09 (12) | C8—C7—C6 | 115.23 (14) |
| O2—C2—C1 | 123.77 (14) | C8—C7—C9 | 121.90 (14) |
| O2—C2—C3 | 131.48 (15) | C3—C8—N1 | 110.23 (13) |
| C3—C2—C1 | 104.74 (12) | C7—C8—N1 | 126.90 (14) |
| C4—C3—C2 | 132.06 (14) | C7—C8—C3 | 122.87 (14) |
| C4—C3—C8 | 120.39 (14) | C7—C9—H9A | 109.5 |
| C8—C3—C2 | 107.47 (13) | C7—C9—H9B | 109.5 |
| C3—C4—H4 | 121.0 | C7—C9—H9C | 109.5 |
| C5—C4—C3 | 118.09 (14) | H9A—C9—H9B | 109.5 |
| C5—C4—H4 | 121.0 | H9A—C9—H9C | 109.5 |
| C4—C5—H5 | 119.8 | H9B—C9—H9C | 109.5 |
| C4—C5—C6 | 120.40 (15) | | |
| | | | |
| O1—C1—C2—O2 | 2.2 (3) | C3—C4—C5—C6 | −0.1 (2) |
| O1—C1—C2—C3 | −176.68 (16) | C4—C3—C8—N1 | −178.04 (14) |
| O2—C2—C3—C4 | −2.8 (3) | C4—C3—C8—C7 | 1.0 (2) |
| O2—C2—C3—C8 | −179.42 (17) | C4—C5—C6—C7 | 0.9 (3) |
| N1—C1—C2—O2 | −179.03 (16) | C5—C6—C7—C8 | −0.7 (2) |
| N1—C1—C2—C3 | 2.08 (16) | C5—C6—C7—C9 | 178.84 (15) |
| C1—N1—C8—C3 | 2.46 (18) | C6—C7—C8—N1 | 178.62 (14) |
| C1—N1—C8—C7 | −176.57 (15) | C6—C7—C8—C3 | −0.3 (2) |
| C1—C2—C3—C4 | 175.98 (16) | C8—N1—C1—O1 | 175.98 (16) |
| C1—C2—C3—C8 | −0.66 (16) | C8—N1—C1—C2 | −2.74 (17) |
| C2—C3—C4—C5 | −177.07 (16) | C8—C3—C4—C5 | −0.8 (2) |
| C2—C3—C8—N1 | −0.94 (17) | C9—C7—C8—N1 | −0.9 (2) |
| C2—C3—C8—C7 | 178.13 (14) | C9—C7—C8—C3 | −179.79 (14) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.88 (1) | 2.03 (1) | 2.8907 (17) | 170 (2) |

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