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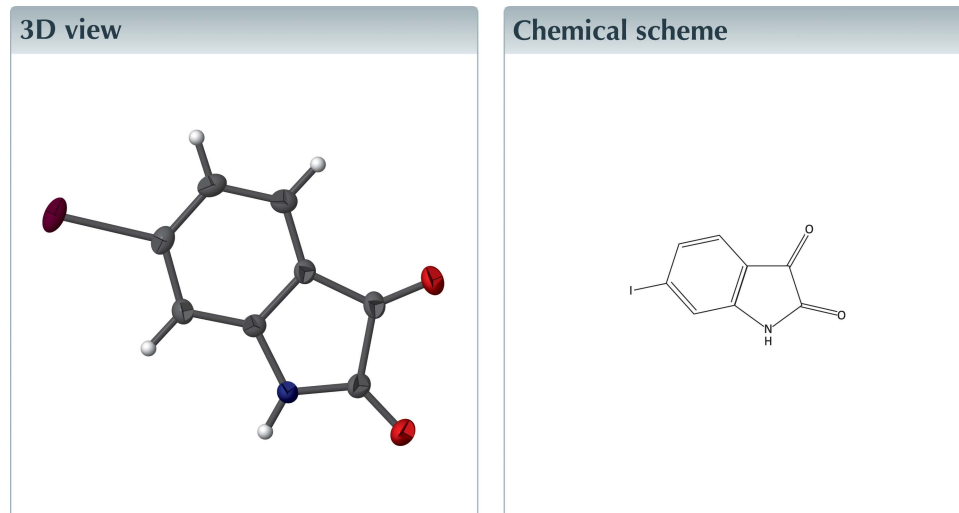
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

## 6-Iodo-1*H*-indole-2,3-dione

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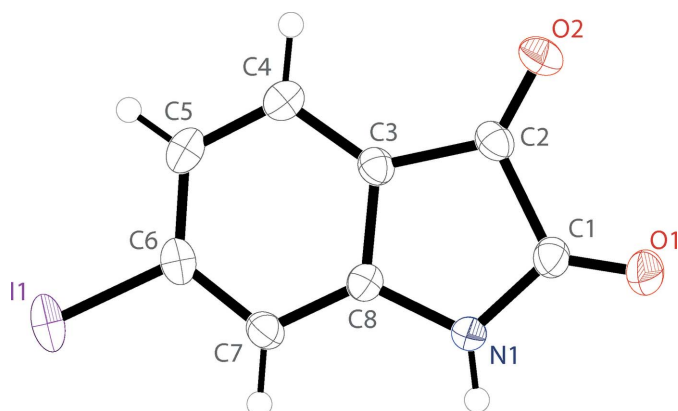
The molecule of the title compound,  $C_8H_4INO_2$ , is almost planar, having an r.m.s. deviation from planarity of 0.019 Å for all non-H atoms. In the crystal, molecules are linked by pairs of  $N-H\cdots O$  hydrogen bonds, forming inversion dimers with an  $R_2^2(8)$  ring motif. The dimers are further linked by  $I\cdots O$  close contacts of 3.078 (2) Å, forming chains along  $[10\bar{1}]$ . The nine-membered fused rings of the isatin molecules stack along the  $b$  axis, with parallel slipped  $\pi$ – $\pi$  interactions [intercentroid distance = 3.594 (2) Å, interplanar distance = 3.379 (1) Å and slippage = 1.243 Å]. These interactions lead to the formation of a three-dimensional network.



### Structure description

In a continuing study of the structure of halogenated isatins, we report herein on the crystal structure of 6-iodoisatin (Fig. 1). The molecule possesses bond lengths and angles similar to those observed in the parent isatin (Goldschmidt & Llewellyn, 1950). The isatins dimerize in the solid state through pairs  $N1-H1\cdots O1$  hydrogen bonds, forming inversion dimers with an  $R_2^2(8)$  ring motif. These dimers are further linked through  $I1\cdots O1$  close contacts of 3.078 (2) Å that result in infinite chains along  $[10\bar{1}]$ ; see Fig. 2 and Table 1. The nine-membered fused rings of the isatin stack along  $b$  with parallel slipped  $\pi$ – $\pi$  interactions [ $Cg2\cdots Cg1^i = 3.594$  (2) Å, inter-planar distance: 3.379 (1) Å, slippage: 1.243 Å;  $Cg1$  and  $Cg2$  are the centroids of rings  $N1/C1-C3/C8$  and  $C3-C8$ , respectively; symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ ]. The result of these interactions is the formation of a three-dimensional network.

The  $I\cdots O$  close contacts reported in the title compound are observed in the other three isomers of iodoisatin (Garden *et al.*, 2006; Golen & Manke, 2016*a,b*). The crystal structure of 6-bromoisatin (Turbitt *et al.*, 2016) also exhibits a similar halogen–oxygen interaction.



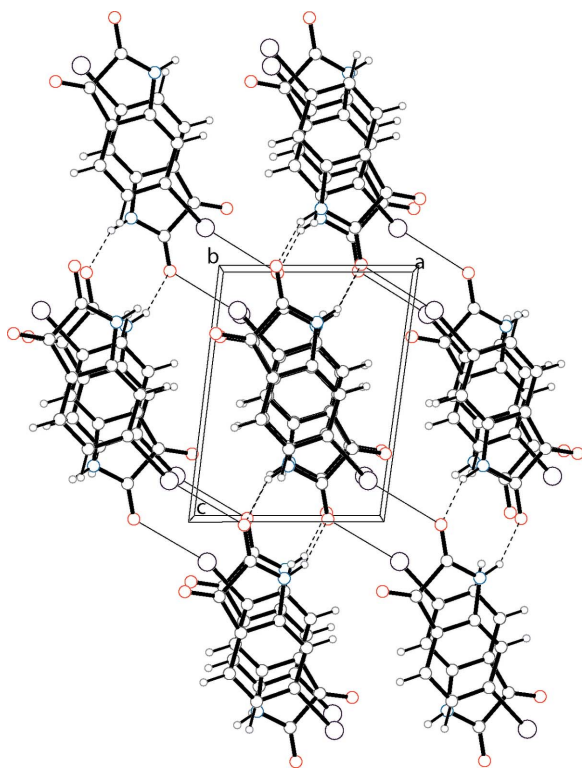
**Figure 1**  
Molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

### Synthesis and crystallization

A commercial sample (Matrix Scientific) of 6-iodo-1*H*-indole-2,3-dione was used for crystallization. A sample suitable for single-crystal X-ray analysis was grown from the slow evaporation of an acetone solution.

### Refinement

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



**Figure 2**  
Crystal packing of the title compound viewed along the *b* axis, with hydrogen bonds shown as dashed lines (see Table 1), and Iodine-oxygen interactions shown as thin solid lines.

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

<i>D</i> – <i>H</i> ··· <i>A</i>	<i>D</i> – <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> – <i>H</i> ··· <i>A</i>
<i>N</i> 1– <i>H</i> 1··· <i>O</i> 1 <sup>i</sup>	0.87 (1)	2.10 (2)	2.888 (3)	152 (3)

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$C_8H_4INO_2$
<i>M<sub>r</sub></i>	273.02
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	200
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.4152 (12), 7.5089 (12), 8.9546 (15)
$\alpha$ , $\beta$ , $\gamma$ (°)	110.162 (7), 96.120 (8), 91.997 (8)
<i>V</i> (Å <sup>3</sup> )	401.43 (12)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	3.94
Crystal size (mm)	0.22 × 0.2 × 0.1
Data collection	
Diffraction	Bruker Venture D8 CMOS
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2014)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.197, 0.259
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	7043, 1533, 1428
<i>R<sub>int</sub></i>	0.030
(sin $\theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.613
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.020, 0.044, 1.13
No. of reflections	1533
No. of parameters	112
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	1.12, -0.74

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

### Acknowledgements

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## full crystallographic data

*IUCrData* (2016). **1**, x160700 [doi:10.1107/S2414314616007008]**6-Iodo-1*H*-indole-2,3-dione**

James A. Golen and David R. Manke

**6-Iodo-1*H*-indole-2,3-dione***Crystal data* $C_8H_4INO_2$  $M_r = 273.02$ Triclinic,  $P\bar{1}$  $a = 6.4152$  (12) Å $b = 7.5089$  (12) Å $c = 8.9546$  (15) Å $\alpha = 110.162$  (7)° $\beta = 96.120$  (8)° $\gamma = 91.997$  (8)° $V = 401.43$  (12) Å<sup>3</sup> $Z = 2$  $F(000) = 256$  $D_x = 2.259$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5053 reflections

 $\theta = 2.9$ – $25.9$ ° $\mu = 3.94$  mm<sup>-1</sup> $T = 200$  K

BLOCK, yellow

 $0.22 \times 0.2 \times 0.1$  mm*Data collection*Bruker Venture D8 CMOS  
diffractometer

Radiation source: Mo

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2014)

 $T_{\min} = 0.197$ ,  $T_{\max} = 0.259$ 

7043 measured reflections

1533 independent reflections

1428 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.030$  $\theta_{\max} = 25.9$ °,  $\theta_{\min} = 2.9$ ° $h = -7 \rightarrow 7$  $k = -9 \rightarrow 9$  $l = -10 \rightarrow 10$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.020$  $wR(F^2) = 0.044$  $S = 1.13$ 

1533 reflections

112 parameters

1 restraint

Hydrogen site location: mixed

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0052P)^2 + 0.5065P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 1.12$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.74$  e Å<sup>-3</sup>*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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.88468 (3)	0.23586 (3)	0.83188 (2)	0.03175 (8)
O1	0.2881 (4)	0.1534 (3)	0.0076 (2)	0.0348 (5)
O2	0.0321 (3)	0.3232 (3)	0.2659 (3)	0.0326 (5)
N1	0.5260 (4)	0.1523 (4)	0.2204 (3)	0.0246 (5)
H1	0.621 (4)	0.087 (4)	0.168 (4)	0.030*
C1	0.3425 (5)	0.1870 (4)	0.1497 (3)	0.0244 (6)
C2	0.2080 (5)	0.2776 (4)	0.2872 (3)	0.0230 (6)
C3	0.3404 (4)	0.2856 (4)	0.4329 (3)	0.0208 (6)
C4	0.3091 (5)	0.3516 (4)	0.5932 (3)	0.0263 (6)
H4	0.1825	0.4068	0.6248	0.032*
C5	0.4653 (5)	0.3358 (4)	0.7071 (3)	0.0275 (7)
H5	0.4460	0.3788	0.8173	0.033*
C6	0.6502 (5)	0.2565 (4)	0.6580 (3)	0.0242 (6)
C7	0.6862 (5)	0.1905 (4)	0.4976 (3)	0.0229 (6)
H7	0.8137	0.1373	0.4662	0.028*
C8	0.5280 (5)	0.2063 (4)	0.3870 (3)	0.0205 (6)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
I1	0.03483 (13)	0.03183 (12)	0.02774 (12)	-0.00684 (8)	-0.01217 (8)	0.01497 (9)
O1	0.0388 (13)	0.0438 (13)	0.0224 (11)	0.0155 (11)	0.0011 (9)	0.0120 (10)
O2	0.0264 (12)	0.0370 (12)	0.0334 (12)	0.0136 (10)	0.0013 (9)	0.0106 (10)
N1	0.0219 (13)	0.0325 (13)	0.0186 (12)	0.0105 (11)	0.0028 (10)	0.0070 (10)
C1	0.0289 (16)	0.0229 (14)	0.0207 (15)	0.0066 (12)	0.0010 (12)	0.0071 (12)
C2	0.0220 (16)	0.0198 (13)	0.0264 (15)	0.0032 (12)	-0.0010 (12)	0.0079 (12)
C3	0.0214 (15)	0.0194 (13)	0.0219 (14)	0.0030 (11)	0.0008 (11)	0.0080 (11)
C4	0.0277 (17)	0.0265 (15)	0.0233 (15)	0.0036 (13)	0.0053 (12)	0.0063 (12)
C5	0.0350 (18)	0.0274 (15)	0.0189 (14)	0.0014 (13)	0.0051 (13)	0.0064 (12)
C6	0.0268 (17)	0.0222 (14)	0.0230 (14)	-0.0027 (12)	-0.0037 (12)	0.0096 (12)
C7	0.0204 (15)	0.0236 (14)	0.0242 (14)	0.0040 (11)	0.0007 (12)	0.0080 (12)
C8	0.0224 (15)	0.0196 (13)	0.0193 (14)	0.0015 (11)	0.0028 (11)	0.0066 (11)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

I1—C6	2.096 (3)	C3—C8	1.400 (4)
O1—C1	1.217 (3)	C4—H4	0.9500
O2—C2	1.206 (3)	C4—C5	1.390 (4)
N1—H1	0.867 (10)	C5—H5	0.9500
N1—C1	1.354 (4)	C5—C6	1.392 (4)
N1—C8	1.403 (4)	C6—C7	1.396 (4)
C1—C2	1.553 (4)	C7—H7	0.9500
C2—C3	1.460 (4)	C7—C8	1.378 (4)
C3—C4	1.388 (4)		

C1—N1—H1	124 (2)	C5—C4—H4	120.4
C1—N1—C8	111.5 (2)	C4—C5—H5	120.4
C8—N1—H1	124 (2)	C4—C5—C6	119.3 (3)
O1—C1—N1	128.2 (3)	C6—C5—H5	120.4
O1—C1—C2	125.7 (3)	C5—C6—I1	118.7 (2)
N1—C1—C2	106.1 (2)	C5—C6—C7	122.6 (3)
O2—C2—C1	123.7 (3)	C7—C6—I1	118.7 (2)
O2—C2—C3	131.6 (3)	C6—C7—H7	121.6
C3—C2—C1	104.7 (2)	C8—C7—C6	116.9 (3)
C4—C3—C2	132.3 (3)	C8—C7—H7	121.6
C4—C3—C8	120.3 (3)	C3—C8—N1	110.3 (2)
C8—C3—C2	107.4 (2)	C7—C8—N1	127.9 (3)
C3—C4—H4	120.4	C7—C8—C3	121.8 (3)
C3—C4—C5	119.2 (3)		
I1—C6—C7—C8	179.9 (2)	C2—C3—C8—C7	-179.2 (3)
O1—C1—C2—O2	0.6 (5)	C3—C4—C5—C6	0.8 (4)
O1—C1—C2—C3	179.2 (3)	C4—C3—C8—N1	-179.1 (3)
O2—C2—C3—C4	-1.8 (6)	C4—C3—C8—C7	0.2 (4)
O2—C2—C3—C8	177.5 (3)	C4—C5—C6—I1	179.6 (2)
N1—C1—C2—O2	-178.5 (3)	C4—C5—C6—C7	-0.2 (4)
N1—C1—C2—C3	0.1 (3)	C5—C6—C7—C8	-0.3 (4)
C1—N1—C8—C3	-1.5 (3)	C6—C7—C8—N1	179.5 (3)
C1—N1—C8—C7	179.2 (3)	C6—C7—C8—C3	0.4 (4)
C1—C2—C3—C4	179.8 (3)	C8—N1—C1—O1	-178.2 (3)
C1—C2—C3—C8	-1.0 (3)	C8—N1—C1—C2	0.8 (3)
C2—C3—C4—C5	178.4 (3)	C8—C3—C4—C5	-0.7 (4)
C2—C3—C8—N1	1.5 (3)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O1 <sup>i</sup>	0.87 (1)	2.10 (2)	2.888 (3)	152 (3)

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