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6-Fluoro-1*H*-indole-2,3-dione

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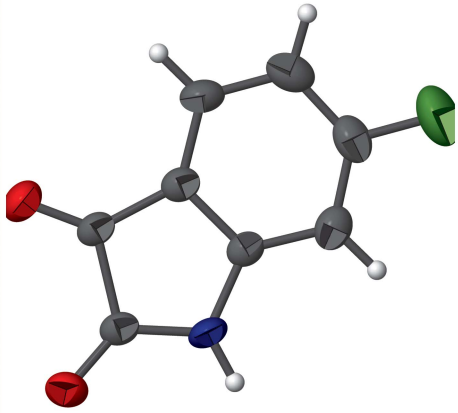
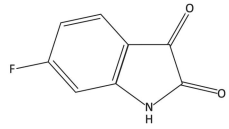
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_8H_4FNO_2$, has a single, almost planar, molecule in the asymmetric unit, with the non-H atoms having a mean deviation from planarity of 0.042 Å. Intermolecular N—H···O hydrogen bonds result in infinite chains along [100]. The molecules are further linked through weak C—H···O and C—H···F interactions.

3D view



Chemical scheme



Structure description

Herein we report the crystal structure of 6-fluoroisatin as part of a continuing study on the structure of halogenated isatins. The structure exhibits a near planar molecule with the non-hydrogen atoms possessing a mean deviation from planarity of 0.042 Å (Fig. 1). The bond lengths and angles were similar to those observed in the parent isatin (Goldschmidt *et al.*, 1950). In the crystal, the molecule exhibits N1—H1···O1 hydrogen bonds that result in infinite chains along [100]. There are also C7—H7···O2 interactions and C5—H5···F1 interactions that further link the molecules in the solid state (Table 1, Fig. 2). These C—H···F interactions are unique to this class of compounds as there are no halogen interactions reported in other fluoroisatin derivatives (Mohamed *et al.*, 2007*a*,*b*; Shankland *et al.*, 2007; Wu *et al.*, 2011; Wang *et al.*, 2012; Mudududdla *et al.*, 2014). The structure of the only other 6-haloisatin reported, 6-bromoisatin, also possesses a halogen interaction, with a Br···O close contact being observed (Turbitt *et al.*, 2016).

Synthesis and crystallization

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

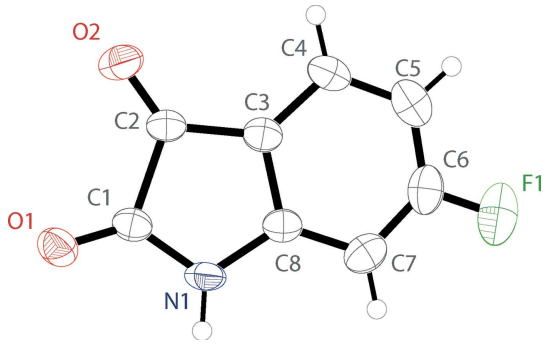


Figure 1
The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

Refinement

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

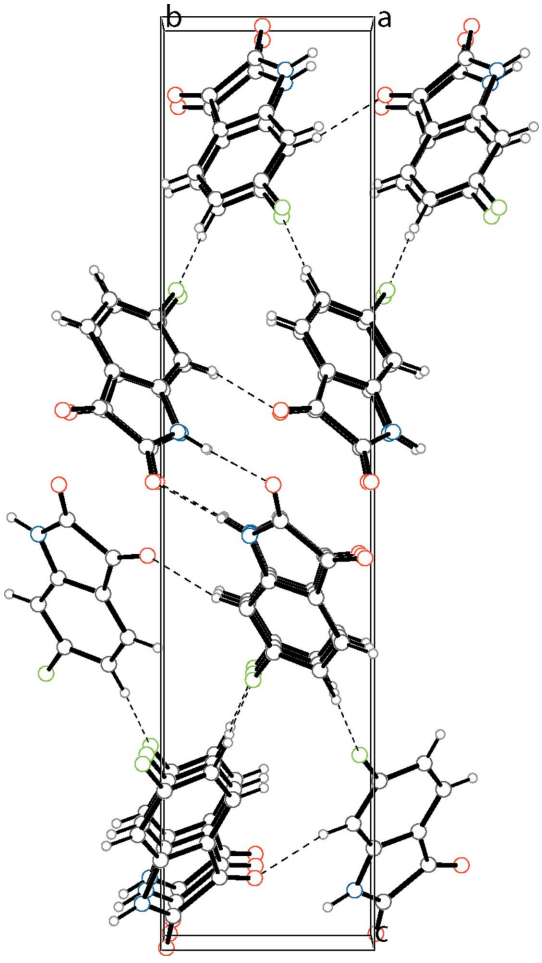


Figure 2
The molecular packing of the title compound, shown along the *a* axis, with hydrogen bonds drawn as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86 (1)	2.03 (1)	2.889 (3)	177 (3)
C5—H5···F1^{ii}	0.93	2.60	3.425 (4)	148
C7—H7···O2^{iii}	0.93	2.36	3.273 (4)	169

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_4FNO_2$
M_r	165.12
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	298
a, b, c (Å)	4.9880 (3), 5.5522 (3), 24.2578 (12)
V (Å^3)	671.80 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.19
Crystal size (mm)	0.25 × 0.15 × 0.1
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.528, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7354, 1205, 1184
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.112, 1.10
No. of reflections	1205
No. of parameters	112
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})	0.49, −0.23
Absolute structure	Flack x determined using 451 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.03 (7)

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160165 [https://doi.org/10.1107/S2414314616001656]

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Crystal data

$C_8H_4FNO_2$
M_r = 165.12
Orthorhombic, $P2_12_12_1$
a = 4.9880 (3) Å
b = 5.5522 (3) Å
c = 24.2578 (12) Å
V = 671.80 (6) Å^3
Z = 4
F(000) = 336
D_x = 1.633 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6268 reflections
θ = 5.5–68.3°
μ = 1.19 mm^{-1}
T = 298 K
BLOCK, orange
0.25 × 0.15 × 0.1 mm

Data collection

Bruker D8 Venture CMOS diffractometer
Radiation source: Cu
HELIOS MX monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.528, T_{max} = 0.753
7354 measured reflections
1205 independent reflections
1184 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 68.3°, θ_{min} = 9.1°
h = −6→5
k = −6→6
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.112
S = 1.10
1205 reflections
112 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.1919P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack x determined using 451 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.03 (7)

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}
F1	0.0765 (5)	0.5676 (5)	0.70923 (9)	0.0721 (7)
O1	1.0503 (4)	0.4748 (4)	0.50142 (8)	0.0409 (5)
O2	1.0523 (4)	0.0601 (4)	0.57698 (9)	0.0438 (6)
N1	0.6855 (5)	0.5829 (4)	0.55480 (9)	0.0345 (6)
H1	0.644 (7)	0.712 (4)	0.5368 (11)	0.041*
C1	0.8919 (5)	0.4412 (5)	0.53884 (10)	0.0317 (6)
C2	0.8971 (6)	0.2246 (4)	0.57986 (10)	0.0310 (6)
C3	0.6835 (5)	0.2782 (5)	0.61916 (10)	0.0327 (6)
C4	0.6008 (7)	0.1608 (5)	0.66655 (11)	0.0398 (7)
H4	0.6838	0.0190	0.6777	0.048*
C5	0.3914 (7)	0.2583 (6)	0.69712 (12)	0.0467 (7)
H5	0.3297	0.1827	0.7289	0.056*
C6	0.2774 (6)	0.4711 (7)	0.67891 (11)	0.0432 (7)
C7	0.3538 (6)	0.5951 (6)	0.63205 (12)	0.0398 (7)
H7	0.2705	0.7371	0.6211	0.048*
C8	0.5624 (5)	0.4936 (5)	0.60257 (10)	0.0308 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0613 (12)	0.0928 (17)	0.0622 (12)	0.0084 (15)	0.0169 (10)	−0.0181 (12)
O1	0.0407 (11)	0.0395 (10)	0.0426 (10)	−0.0048 (9)	0.0053 (8)	0.0086 (9)
O2	0.0450 (11)	0.0342 (10)	0.0522 (11)	0.0089 (10)	−0.0021 (9)	0.0043 (9)
N1	0.0393 (12)	0.0250 (11)	0.0394 (12)	0.0020 (10)	−0.0016 (10)	0.0107 (9)
C1	0.0330 (12)	0.0272 (12)	0.0348 (12)	−0.0046 (11)	−0.0039 (10)	0.0040 (10)
C2	0.0329 (12)	0.0251 (12)	0.0349 (12)	−0.0017 (12)	−0.0048 (11)	0.0026 (10)
C3	0.0345 (13)	0.0290 (13)	0.0346 (13)	−0.0024 (12)	−0.0036 (11)	0.0027 (10)
C4	0.0482 (16)	0.0348 (14)	0.0365 (13)	−0.0038 (14)	−0.0022 (14)	0.0090 (11)
C5	0.0508 (17)	0.0541 (16)	0.0354 (13)	−0.0104 (18)	0.0032 (13)	0.0026 (13)
C6	0.0373 (14)	0.0546 (19)	0.0377 (14)	−0.0023 (14)	0.0031 (11)	−0.0128 (13)
C7	0.0388 (16)	0.0349 (14)	0.0458 (14)	0.0032 (13)	−0.0060 (13)	−0.0059 (11)
C8	0.0321 (13)	0.0265 (12)	0.0337 (12)	−0.0022 (11)	−0.0055 (10)	0.0006 (10)

Geometric parameters (Å, º)

F1—C6	1.353 (4)	C3—C8	1.399 (4)
O1—C1	1.218 (3)	C4—H4	0.9300
O2—C2	1.199 (3)	C4—C5	1.391 (5)
N1—H1	0.864 (13)	C5—H5	0.9300
N1—C1	1.352 (4)	C5—C6	1.383 (5)
N1—C8	1.402 (3)	C6—C7	1.382 (4)
C1—C2	1.561 (3)	C7—H7	0.9300
C2—C3	1.460 (4)	C7—C8	1.383 (4)
C3—C4	1.384 (4)		

C1—N1—H1	121 (2)	C5—C4—H4	120.5
C1—N1—C8	111.4 (2)	C4—C5—H5	121.0
C8—N1—H1	127 (2)	C6—C5—C4	118.1 (3)
O1—C1—N1	128.2 (2)	C6—C5—H5	121.0
O1—C1—C2	125.6 (2)	F1—C6—C5	118.0 (3)
N1—C1—C2	106.2 (2)	F1—C6—C7	117.0 (3)
O2—C2—C1	124.1 (2)	C7—C6—C5	125.1 (3)
O2—C2—C3	131.6 (2)	C6—C7—H7	122.3
C3—C2—C1	104.3 (2)	C6—C7—C8	115.5 (3)
C4—C3—C2	131.6 (3)	C8—C7—H7	122.3
C4—C3—C8	120.8 (3)	C3—C8—N1	110.6 (2)
C8—C3—C2	107.5 (2)	C7—C8—N1	127.8 (3)
C3—C4—H4	120.5	C7—C8—C3	121.6 (2)
C3—C4—C5	118.9 (3)		

F1—C6—C7—C8	179.0 (2)	C2—C3—C8—C7	−179.1 (2)
O1—C1—C2—O2	−3.9 (4)	C3—C4—C5—C6	−0.8 (4)
O1—C1—C2—C3	175.1 (3)	C4—C3—C8—N1	177.9 (2)
O2—C2—C3—C4	3.0 (5)	C4—C3—C8—C7	−1.1 (4)
O2—C2—C3—C8	−179.4 (3)	C4—C5—C6—F1	−179.0 (3)
N1—C1—C2—O2	178.2 (3)	C4—C5—C6—C7	0.6 (5)
N1—C1—C2—C3	−2.8 (3)	C5—C6—C7—C8	−0.6 (5)
C1—N1—C8—C3	−1.9 (3)	C6—C7—C8—N1	−177.9 (3)
C1—N1—C8—C7	177.0 (3)	C6—C7—C8—C3	0.8 (4)
C1—C2—C3—C4	−176.0 (3)	C8—N1—C1—O1	−175.0 (3)
C1—C2—C3—C8	1.7 (3)	C8—N1—C1—C2	2.8 (3)
C2—C3—C4—C5	178.4 (3)	C8—C3—C4—C5	1.1 (4)
C2—C3—C8—N1	−0.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86 (1)	2.03 (1)	2.889 (3)	177 (3)
C5—H5···F1^{ii}	0.93	2.60	3.425 (4)	148
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Symmetry codes: (i) $x-1/2, -y+3/2, -z+1$; (ii) $-x, y-1/2, -z+3/2$; (iii) $x-1, y+1, z$.