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2-Iodobenzaldehyde

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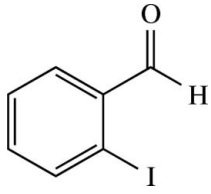
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.006 Å; R factor = 0.025; wR factor = 0.049; data-to-parameter ratio = 19.4.

In the title compound, C_7H_5IO, the intramolecular bond lengths and angles are normal. Non-crystallographic C_s symmetry is broken by a 10.4 (2)° interplanar angle between the formyl group and the aromatic plane. The shortest intermolecular contact [I···O = 3.124 (3) Å; 0.38 Å shorter than the sum of the respective van der Waals radii] reveals the presence of a dispersive I···O attraction.

Related literature

For the synthesis of the title compound, see Angyal *et al.* (1949). For the crystal structure of a related compound in which iodine atoms are present in close proximity to the formyl group, see: Matos Beja *et al.* (2002).



Experimental

Crystal data

C_7H_5IO
M_r = 232.01
Orthorhombic, $P2_12_12_1$
a = 4.1213 (5) Å
b = 11.4948 (12) Å
c = 14.8310 (14) Å
V = 702.60 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.47 mm^{-1}
T = 200 (2) K
0.29 × 0.11 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.597, T_{max} = 0.866
4122 measured reflections
1614 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.049
S = 0.98
1614 reflections
83 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}
Absolute structure: Flack (1983); 635 Friedel pairs
Flack parameter: 0.003 (45)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2365).

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supplementary materials

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2-Iodobenzaldehyde

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Comment

The title compound (I) was prepared as an intermediate in the synthesis of *ortho*-iodomandelic acid.

In the molecule, the formyl group is almost coplanar to the aromatic system but is tilted by about 10° with respect to the aromatic ring. This value is markedly smaller than the same angle in the sterically overloaded di-iodo derivative described by Matos Beja *et al.* (2002). The H atom of the formyl group is oriented to the I atom (Fig. 1). Bond lengths and angles are normal (Matos Beja *et al.*, 2002).

In terms of van-der-Waals radii, the shortest intermolecular contact stems from an obviously dispersive attraction between iodine and oxygen atoms (0.38 Å less than the sum of vdW radii). Other intermolecular contacts are outside the van-der-Waals surface of the individual atoms.

Experimental

The title compound was obtained as an intermediate in the synthesis of *ortho*-iodomandelic acid according to a published procedure (Angyal *et al.*, 1949) upon decomposition of the hexamine salt of 2-iodobenzyl bromide under aqueous acidic conditions. Crystals suitable for X-ray analysis were obtained by recrystallization of the compound from boiling *n*-pentane.

Refinement

All H atoms were located in a difference map and refined as riding on their parent atoms. One common isotropic displacement parameter for all H atoms was refined to 0.048 (6).

Figures

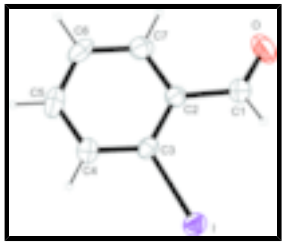

Fig. 1. The molecular structure of (I), with atom labels and anisotropic displacement ellipsoids drawn at the 50% probability level for non-H atoms.

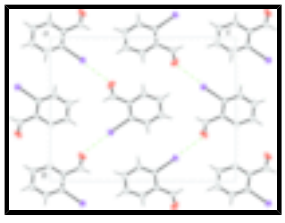

Fig. 2. The packing of (I), viewed along [−1 0 0]. Dotted green lines denote short iodine···oxygen contacts.

2-Iodobenzaldehyde

Crystal data

C_7H_5IO	F_{000} = 432
M_r = 232.01	D_x = 2.193 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	θ = 3.8–27.5º
a = 4.1213 (5) Å	μ = 4.47 mm^{-1}
b = 11.4948 (12) Å	T = 200 (2) K
c = 14.8310 (14) Å	Platelet, colourless
V = 702.60 (13) Å^3	0.29 × 0.11 × 0.04 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1614 independent reflections
Radiation source: fine-focus sealed tube	1486 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.050
T = 200(2) K	θ_{max} = 27.5º
ω–scans	θ_{min} = 3.8º
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	h = −5→2
T_{min} = 0.597, T_{max} = 0.866	k = −14→14
4122 measured reflections	l = −19→18

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$w = 1/[\sigma^2(F_o^2) + (0.0187P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.049	$(\Delta/\sigma)_{max} < 0.001$
S = 0.98	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
1614 reflections	$\Delta\rho_{min}$ = −0.87 e Å^{-3}
83 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983); 635 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.003 (45)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
I	−0.20356 (6)	−0.15824 (2)	0.674261 (19)	0.02777 (8)

O	0.4098 (8)	0.1724 (3)	0.6713 (2)	0.0490 (9)
C1	0.2202 (11)	0.0923 (3)	0.6618 (3)	0.0324 (9)
H1	0.1275	0.0586	0.7143	0.048 (6)*
C2	0.1259 (10)	0.0447 (4)	0.5732 (3)	0.0241 (9)
C3	−0.0529 (10)	−0.0579 (3)	0.5630 (3)	0.0241 (9)
C4	−0.1329 (10)	−0.0984 (4)	0.4781 (3)	0.0295 (10)
H4	−0.2512	−0.1688	0.4717	0.048 (6)*
C5	−0.0413 (11)	−0.0367 (4)	0.4026 (3)	0.0353 (11)
H5	−0.0973	−0.0648	0.3445	0.048 (6)*
C6	0.1309 (11)	0.0655 (4)	0.4108 (3)	0.0328 (11)
H6	0.1890	0.1086	0.3586	0.048 (6)*
C7	0.2193 (11)	0.1051 (3)	0.4958 (3)	0.0298 (9)
H7	0.3446	0.1741	0.5014	0.048 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I	0.02795 (13)	0.02990 (12)	0.02547 (12)	−0.00281 (11)	0.00231 (11)	0.00323 (13)
O	0.064 (2)	0.0406 (18)	0.0419 (19)	−0.0213 (16)	0.0052 (19)	−0.0156 (19)
C1	0.041 (2)	0.0304 (19)	0.025 (2)	−0.001 (2)	0.001 (2)	−0.0025 (18)
C2	0.027 (2)	0.0211 (18)	0.024 (2)	0.0036 (17)	0.0032 (17)	−0.0006 (16)
C3	0.024 (2)	0.026 (2)	0.022 (2)	0.0040 (17)	−0.0006 (18)	0.0033 (18)
C4	0.030 (2)	0.034 (2)	0.025 (2)	0.0001 (19)	−0.0025 (18)	−0.002 (2)
C5	0.037 (3)	0.049 (3)	0.020 (2)	0.014 (2)	−0.0025 (19)	−0.004 (2)
C6	0.038 (3)	0.036 (2)	0.025 (2)	0.011 (2)	0.0051 (19)	0.012 (2)
C7	0.033 (2)	0.0251 (17)	0.031 (2)	0.005 (2)	0.006 (2)	−0.0002 (18)

Geometric parameters (Å, °)

I—C3	2.108 (4)	C4—C5	1.377 (6)
O—C1	1.215 (5)	C4—H4	0.9500
C1—C2	1.476 (6)	C5—C6	1.377 (7)
C1—H1	0.9500	C5—H5	0.9500
C2—C7	1.395 (6)	C6—C7	1.389 (6)
C2—C3	1.398 (6)	C6—H6	0.9500
C3—C4	1.382 (6)	C7—H7	0.9500
I···O^{i}	3.124 (3)		
O—C1—C2	123.6 (4)	C3—C4—H4	120.0
O—C1—H1	118.2	C6—C5—C4	120.6 (4)
C2—C1—H1	118.2	C6—C5—H5	119.7
C7—C2—C3	118.4 (4)	C4—C5—H5	119.7
C7—C2—C1	118.3 (4)	C5—C6—C7	119.6 (4)
C3—C2—C1	123.2 (4)	C5—C6—H6	120.2
C4—C3—C2	120.5 (4)	C7—C6—H6	120.2
C4—C3—I	117.3 (3)	C6—C7—C2	120.7 (4)
C2—C3—I	122.1 (3)	C6—C7—H7	119.7
C5—C4—C3	120.1 (4)	C2—C7—H7	119.7
C5—C4—H4	120.0		

O—C1—C2—C7	−10.1 (6)	I—C3—C4—C5	180.0 (3)
O—C1—C2—C3	170.0 (4)	C3—C4—C5—C6	0.1 (6)
C7—C2—C3—C4	0.4 (6)	C4—C5—C6—C7	1.5 (6)
C1—C2—C3—C4	−179.8 (4)	C5—C6—C7—C2	−2.2 (7)
C7—C2—C3—I	179.2 (3)	C3—C2—C7—C6	1.3 (6)
C1—C2—C3—I	−0.9 (6)	C1—C2—C7—C6	−178.6 (4)
C2—C3—C4—C5	−1.1 (6)		

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+3/2.

Fig. 1

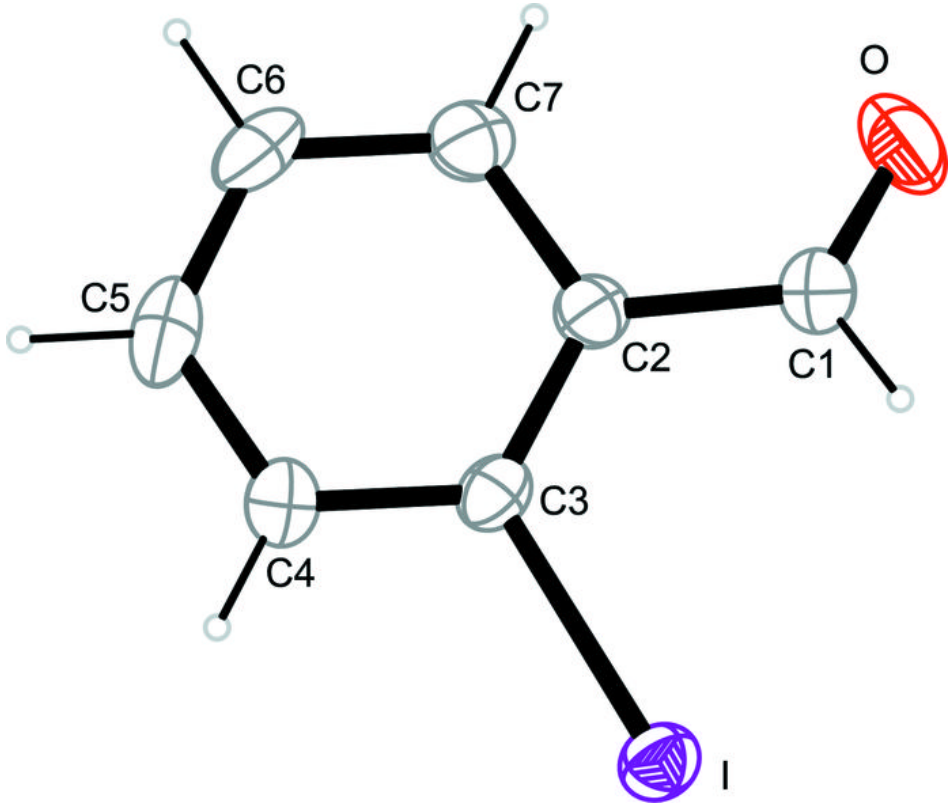

Fig. 2