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1-Bromomethyl-2-iodobenzene

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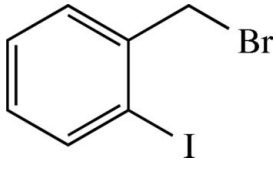
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.005 Å; R factor = 0.024; wR factor = 0.056; data-to-parameter ratio = 22.2.

The title compound, C_7H_6BrI, is a synthon for the transfer of the 2-iodophenyl residue. Bond lengths and angles are normal, the conformation being characterized by an almost perpendicular arrangement of the $C_{ipso}-CH_2-Br$ plane and the plane of the aromatic ring. Instead of halogen–π interactions, the crystal structure is dictated by I···Br van-der Waals contacts [3.6943 (5) Å] and lateral contacts of parallel aromatic residues at a distance of 3.423 Å.

Related literature

For the synthesis of the title compound, see: Bacon & Lindsay (1958). For a related structure, see: Kirsop *et al.* (2006). Swierczynski *et al.* (2005) describe the general significance of halogen–π-system interactions.



Experimental

Crystal data

C_7H_6BrI
M_r = 296.93
Monoclinic, $P2_1/c$
a = 8.7569 (2) Å
b = 12.0237 (4) Å
c = 8.5351 (3) Å
β = 114.777 (2)°
V = 815.94 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.73 mm^{-1}
T = 200 (2) K
0.11 × 0.09 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.398, T_{max} = 0.497
13178 measured reflections
1867 independent reflections
1514 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.056
S = 1.09
1867 reflections
84 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor 1997); 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: *SHELXL97* and Spek (2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2334).

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supplementary materials

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1-Bromomethyl-2-iodobenzene

R. Betz and P. Klüfers

Comment

1-Bromomethyl-2-iodobenzene (*ortho*-iodo-benzylbromide) was prepared as an intermediate in the synthesis of *ortho*-iodomandelic acid. The structure of the compound had been deduced upon spectroscopic data so far.

Bond lengths and angles correspond to the typical values for similar compounds. The angle between the C1—C7—Br plane and the plane of the phenyl carbons is 85.5 (3)°.

In agreement with the low melting point of the title compound of about 55 °C, the crystal structure is determined by van-der-Waals interactions. The most significant interaction in terms of a *PLATON* analysis (Spek, 1990) of the van-der-Waals bond distances are Br···I contacts along [0 1 0]. The phenyl rings are arranged parallel to each other and appear as π-stacked in terms of a 3.423-Å perpendicular distance (red arrows in Fig. 2). However, the mutual overlap of the rings is restricted to a single carbon–carbon bond. Though attractive intermolecular contacts between a halogen atom and a π system are common (Swierczynski *et al.*, 2005), they are not observed in (I).

Experimental

The title compound was prepared according to a published procedure (Bacon & Lindsay, 1958) upon radical-supported bromination of 2-iodotoluene in tetrachloromethane.

Crystals suitable for X-ray analysis were obtained directly from the crystallized reaction product isolated by means of distillation from the reaction mixture.

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.

Figures

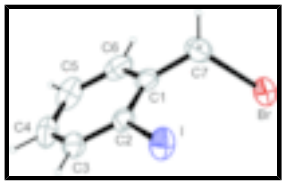

Fig. 1. The molecular structure of (I), with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

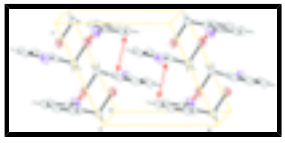

Fig. 2. The packing of (I) in a view close to [0 1 0]. The most significant intermolecular interactions are drawn in red: Br···I contacts that are about 0.1 Å shorter than the sum of the van-der-Waals radii (dots), and 3.4-Å contacts between the rims of parallel phenyl residues (double arrows).

1-Bromomethyl-2-iodobenzene

Crystal data

C_7H_6BrI	F_{000} = 544
M_r = 296.93	D_x = 2.417 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 55 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.7569 (2) Å	Cell parameters from 8472 reflections
b = 12.0237 (4) Å	θ = 3.1–27.5º
c = 8.5351 (3) Å	μ = 8.73 mm^{-1}
β = 114.777 (2)º	T = 200 (2) K
V = 815.94 (5) Å^3	Block, colourless
Z = 4	0.11 × 0.09 × 0.08 mm

Data collection

KappaCCD diffractometer	1867 independent reflections
Radiation source: rotating anode	1514 reflections with $I > 2\sigma(I)$
Monochromator: MONTEL, graded multilayered X-ray optics	R_{int} = 0.032
T = 200(2) K	θ_{max} = 27.5º
ω–scan	θ_{min} = 3.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	h = −11→11
T_{min} = 0.398, T_{max} = 0.497	k = −15→15
13178 measured reflections	l = −11→11

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	Only H-atom displacement parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.024	$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 0.4328P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.056	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.09	$\Delta\rho_{max}$ = 1.05 e Å^{-3}
1867 reflections	$\Delta\rho_{min}$ = −0.58 e Å^{-3}
84 parameters	Extinction correction: SHELXL
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0034 (3)
Secondary atom site location: difference Fourier map	

Special details

Refinement. refU for hydrogen atoms: one common isotropic U for all H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I	0.76744 (3)	0.499318 (17)	0.15316 (3)	0.04592 (11)
Br	1.17131 (4)	0.30304 (3)	0.28843 (4)	0.04037 (12)
C1	0.8186 (4)	0.2499 (3)	0.1176 (4)	0.0325 (7)
C2	0.7165 (3)	0.3295 (2)	0.1485 (4)	0.0307 (6)
C3	0.5795 (4)	0.2968 (3)	0.1788 (4)	0.0367 (7)
H3	0.5108	0.3515	0.1978	0.053 (4)*
C4	0.5423 (4)	0.1859 (3)	0.1815 (4)	0.0432 (8)
H4	0.4485	0.1640	0.2028	0.053 (4)*
C5	0.6414 (4)	0.1067 (3)	0.1530 (4)	0.0459 (8)
H5	0.6166	0.0300	0.1562	0.053 (4)*
C6	0.7761 (4)	0.1380 (3)	0.1202 (4)	0.0415 (8)
H6	0.8419	0.0823	0.0988	0.053 (4)*
C7	0.9624 (4)	0.2805 (3)	0.0772 (4)	0.0448 (8)
H71	0.9349	0.3498	0.0080	0.053 (4)*
H72	0.9806	0.2209	0.0068	0.053 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I	0.03819 (15)	0.03381 (16)	0.06009 (18)	−0.00073 (8)	0.01501 (12)	0.00094 (10)
Br	0.02986 (17)	0.0446 (2)	0.0481 (2)	−0.00055 (14)	0.01776 (14)	0.00128 (16)
C1	0.0297 (14)	0.0391 (18)	0.0231 (15)	0.0033 (13)	0.0056 (12)	−0.0024 (12)
C2	0.0270 (13)	0.0325 (16)	0.0268 (14)	0.0022 (12)	0.0055 (11)	−0.0004 (12)
C3	0.0277 (14)	0.0436 (19)	0.0352 (16)	0.0028 (13)	0.0096 (12)	−0.0013 (14)
C4	0.0305 (15)	0.048 (2)	0.0440 (19)	−0.0097 (14)	0.0083 (14)	0.0045 (16)
C5	0.0412 (18)	0.0363 (19)	0.0441 (19)	−0.0057 (15)	0.0022 (14)	0.0029 (16)
C6	0.0404 (17)	0.039 (2)	0.0325 (17)	0.0094 (14)	0.0025 (14)	−0.0098 (14)
C7	0.0368 (17)	0.065 (2)	0.0339 (17)	0.0104 (16)	0.0164 (14)	0.0043 (16)

Geometric parameters (Å, °)

I—C2	2.087 (3)	C4—C5	1.377 (5)
Br—C7	1.977 (3)	C4—H4	0.9500
C1—C6	1.400 (5)	C5—C6	1.374 (5)
C1—C2	1.408 (4)	C5—H5	0.9500
C1—C7	1.484 (4)	C6—H6	0.9500
C2—C3	1.385 (4)	C7—H71	0.9900
C3—C4	1.376 (5)	C7—H72	0.9900
C3—H3	0.9500		
Br···I^{i}	3.6943 (5)		

C6—C1—C2	117.1 (3)	C6—C5—C4	120.3 (3)
C6—C1—C7	120.0 (3)	C6—C5—H5	119.8
C2—C1—C7	122.9 (3)	C4—C5—H5	119.8
C3—C2—C1	120.7 (3)	C5—C6—C1	121.6 (3)
C3—C2—I	117.9 (2)	C5—C6—H6	119.2
C1—C2—I	121.4 (2)	C1—C6—H6	119.2
C4—C3—C2	120.5 (3)	C1—C7—Br	111.9 (2)
C4—C3—H3	119.7	C1—C7—H71	109.2
C2—C3—H3	119.7	Br—C7—H71	109.2
C3—C4—C5	119.8 (3)	C1—C7—H72	109.2
C3—C4—H4	120.1	Br—C7—H72	109.2
C5—C4—H4	120.1	H71—C7—H72	107.9
C6—C1—C2—C3	−0.4 (4)	C3—C4—C5—C6	−0.7 (5)
C7—C1—C2—C3	177.3 (3)	C4—C5—C6—C1	1.2 (5)
C6—C1—C2—I	178.8 (2)	C2—C1—C6—C5	−0.6 (4)
C7—C1—C2—I	−3.4 (4)	C7—C1—C6—C5	−178.4 (3)
C1—C2—C3—C4	0.9 (4)	C6—C1—C7—Br	−95.8 (3)
I—C2—C3—C4	−178.4 (2)	C2—C1—C7—Br	86.4 (3)
C2—C3—C4—C5	−0.3 (5)		

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

Fig. 1

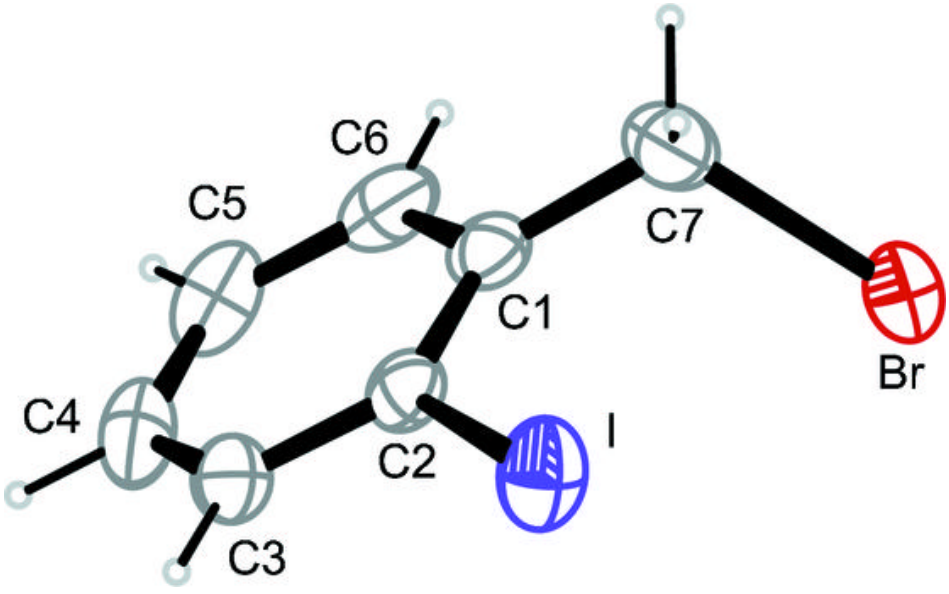

Fig. 2