research papers

C—I⋯N and C—I⋯π halogen bonding in the structures of 1-benzyliodoimidazole derivatives

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Halogen bonding is a well-established and intensively studied intermolecular interaction that has also been used in the preparation of functional materials. While polyfluoroiodo- and polyfluorobromobenzenes have been widely used as aromatic halogen-bond donors, there have been very few studies of iodo-imidazoles with regard to halogen bonding. We describe here the X-ray structures of three iodoimidazole derivatives, namely 1-benzyl-2-iodo-1H-imidazole, $C_{10}H_9IN_2$, (1), 1-benzyl-4-iodo-1H-imidazole, $C_{10}H_9IN_2$, (2), and 1-benzyl-2-iodo-1H-benzimidazole, $C_{14}H_{11}IN_2$, (3), and the halogen bonds that dominate the intermolecular interactions in each of these three structures. The three-dimensional structure of (1) is dominated by a strong C—I⋯N halogen bond, with an N⋯I distance of 2.8765 (2) Å, that connects the molecules into one-dimensional zigzag ribbons of molecules. In contrast, the three-dimensional structures of (2) and (3) both feature C—I⋯π halogen-bonded dimers.

1. Introduction

Halogen bonding is now a well-established and intensively studied intermolecular interaction that has also been used in the preparation of functional materials (Cavallo *et al.*, 2016; Gilday *et al.*, 2015). While polyfluoroiodo- and polyfluorobromobenzenes have been widely used as aromatic halogen-bond donors, there have been very few studies of iodo-imidazoles with regard to halogen bonding. Indeed, a search of the Cambridge Structural Database (CSD; Version 5.37; Groom *et al.*, 2016) using *Conquest* (Bruno *et al.*, 2002) revealed 74 examples involving iodoimidazoles. It is note-worthy, however, that only 18 of the 74 structures contained neutral iodinated imidazole derivatives. Furthermore, 14 of these 18 structures do not exhibit any close contacts to the I atoms. The structures of five neutral N-unsubstituted iodo-imidazoles are dominated by N—H⋯N hydrogen bonds [refcodes BOWREM, BOWRUC and BOWSAJ (Andrze-jewski *et al.*, 2015), GARJUG (Chlupatý *et al.*, 2012), and WISBUL (Ding *et al.*, 2012)] and one structure features N—H⋯O hydrogen bonds (KOZLIW; Jansa *et al.*, 2015), while seven more sterically hindered imidazole derivatives do not display any major intermolecular interactions and the three-dimensional structures presumably have controlled close packing based on size, shape, and polarity [GOGYOR (Delest *et al.*, 2008), IGUANM (Al-Mukhtar & Wilson, 1978), KIRYEQ (Poverlein *et al.*, 2007), UJOCIF (Tschamber *et al.*, 2003), NUCRAE (Phillips *et al.*, 1997), UNIFUS (Terinek & Vasella, 2003), and UXOXOV (Li *et al.*, 2011)]. In contrast, three unhindered N-substituted iodoimidazoles do display C—I⋯N halogen bonding as the major intermolecular interaction [BEQWEB (Mukai & Nishikawa, 2013), GOGYIL
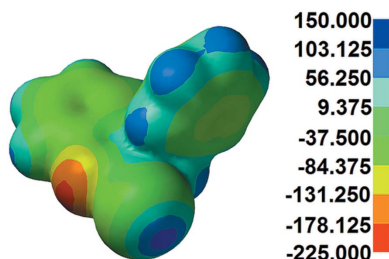

150.000
103.125
56.250
9.375
-37.500
-84.375
-131.250
-178.125
-225.000

Table 1
Experimental details.

	(1)	(2)	(3)
Crystal data			
Chemical formula	$C_{10}H_9IN_2$	$C_{10}H_9IN_2$	$C_{14}H_{11}IN_2$
M_r	284.09	284.09	334.15
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$
Temperature (K)	100	100	100
a, b, c (Å)	8.7561 (5), 9.0016 (5), 12.8869 (7)	8.4574 (5), 6.1526 (3), 19.4261 (10)	6.4606 (8), 8.2346 (10), 12.3451 (14)
α, β, γ (°)	90, 90, 90	90, 96.362 (1), 90	108.064 (1), 94.174 (2), 95.366 (2)
V (Å^3)	1015.73 (10)	1004.61 (9)	618.05 (13)
Z	4	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	3.11	3.14	2.57
Crystal size (mm)	$0.30 \times 0.20 \times 0.05$	$0.22 \times 0.22 \times 0.22$	$0.20 \times 0.20 \times 0.20$
Data collection			
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)	Multi-scan (*SADABS*; Bruker, 2014)	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.622, 0.746	0.594, 0.746	0.588, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13262, 2228, 2202	12374, 2207, 2114	8079, 2777, 2725
R_{int}	0.030	0.021	0.016
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.641	0.641	0.645
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.013, 0.030, 1.05	0.016, 0.037, 1.11	0.015, 0.039, 1.09
No. of reflections	2228	2207	2777
No. of parameters	118	118	154
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.25, −0.27	0.73, −0.52	0.74, −0.35
Absolute structure	See §2.2	–	–

Computer programs: *SMART* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b) and *X-SEED* (Barbour, 2001).

(Delest *et al.*, 2008) and HUDSUW (Byrne, 2015)]. A particularly striking example is the identification of a trimeric halogen-bonded unit by Mukai & Nishikawa (2013). The

(1)

(2)

(3)
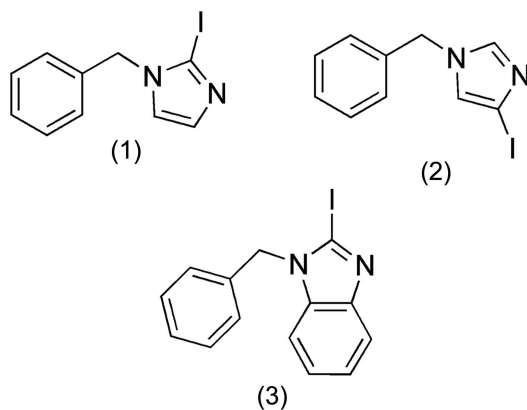
reported halogen bonds have N···I distances between 2.884 and 2.953 Å, corresponding to 81.7–83.7% of the sum of the van der Waals radii of 3.53 Å (Bondi, 1964), and are essentially linear, with C—I···N angles between 171.38 and 174.86°. In this study, we present the structures of three iodoimidazole derivatives, namely 1-benzyl-2-iodo-1H-imidazole, (1), 1-benzyl-4-iodo-1H-imidazole, (2), and 1-benzyl-2-iodo-1H-benzimidazole, (3), and discuss the intermolecular halogen-bonding interactions and other nonbonding interactions that dominate the crystal structures.

2. Experimental

2.1. Synthesis and crystallization

2.1.1. 1-Benzyl-2-iodo-1H-imidazole, (1). 1-Benzyl-1H-imidazole was synthesized according to the procedure of Salvio *et al.* (2011). Compound (1) was synthesized from 1-benzyl-1H-imidazole using a modification of the procedure of de Figueiredo (2007). Thus, 1-benzyl-1H-imidazole (2 g, 12.64 mmol) and anhydrous tetrahydrofuran (35 ml) were added to a three-necked 250 ml round-bottomed flask under an argon atmosphere. The mixture was cooled to 195 K and stirred at this temperature for 7 min. 1.6 M *n*-BuLi (8 ml, 12.64 mmol, 1 equivalent) was added dropwise over a period of 2 mins and the resultant mixture stirred at 195 K for 45 min. Iodine (4.81 g, 18.96 mmol, 1.5 equivalents) was crushed and added to the stirred mixture. The cooling bath was removed and the mixture stirred at room temperature for 3 h under argon. The mixture was extracted with CH_2Cl_2 (300 ml) and the excess I_2 was quenched with 10% Na_2SO_3 (200 ml). The organic layer was separated, washed twice with H_2O (200 ml) and twice with brine (200 ml), and then dried over Na_2SO_4. The solvent was removed *in vacuo* and the crude product purified by flash column chromatography using a 10:1 (*v/v*) mixture of hexane and ethyl acetate to afford 2.23 g of the compound as a white solid (yield 7.85 mmol, 62%). $R_F = 0.27$ (hexane/EtOAc, 2:1 *v/v*). The solid was crystallized from a 9:1 (*v/v*) mixture of hexane and ethyl acetate to give white needle-
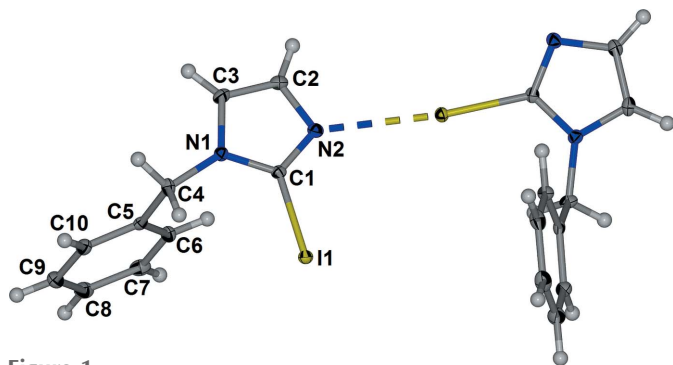
Figure 1
The molecular structure of (1), showing the imidazole N···I halogen bond (dashed line). Displacement ellipsoids for the non-H atoms are drawn at the 50% probability level.

like crystals [m.p. 373.5–375.9 K; literature 372–374 K (Moreno-Manas *et al.*, 1990)]. ^{1}H NMR (400 MHz, CDCl$_3$): δ 5.10 (*s*, 2H), 7.01 (*d*, *J* = 1.6 Hz, 1H), 7.12–7.15 (*m*, 3H), 7.32–7.38 (*m*, 3H).

2.1.2. 1-Benzyl-4-iodo-1*H*-imidazole, (2). Compound (2) was synthesized from commercially available 4-iodo-1*H*-imidazole using a similar procedure to that used to synthesize 1-benzyl-1*H*-imidazole (see *Supporting information*).

2.1.3. 1-Benzyl-2-iodo-1*H*-benzimidazole, (3). 1-Benzyl-1*H*-benzimidazole and the iodinated compound (3) were synthesized using the modified procedure used for the preparation of (1) (see *Supporting information*).

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were treated as riding atoms in geometrically idealized positions, with C—H = 0.95 (aromatic) or 0.98 Å (methylene) and U_{iso}(H) = kU_{iso}(C), where k = 1.5 for the methylene group and 1.2 for all aromatic H atoms. The correct absolute configuration for the molecules of compound (1) in the crystal selected for data collection was determined by the Flack *x* parameter (Flack, 1983) of −0.002 (13) by a classical fit to all intensities and was calculated using 913 quotients $[(I^+) − (I^−)]/[(I^+) + (I^−)]$ (Parsons *et al.*, 2013).

2.3. Electrostatic potential calculations

All molecules were geometry optimized using the *Spartan'10* (Wavefunction, 2010) molecular modeling program

with density functional theory (DFT) at the B3LYP/6-311+G** level, and the corresponding molecular electrostatic potential energy surface was determined also using *Spartan'10*. The initial geometry for the optimization corresponded to that observed in the corresponding crystal structure. In the optimized geometry (gas phase), the benzyl group is rotated relative to the imidazole ring and minor conformation-based differences in the electrostatic potentials may be expected between the two conformations. The differences between the observed conformation and the optimized conformation of each of (1), (2), and (3) are collected in Table S1 in the *Supporting information*.

3. Results and discussion

The asymmetric unit of the X-ray structure of (1) contains a single molecule. The phenyl group is essentially orthogonal to the imidazole group, with a dihedral angle between the planes defined by the phenyl C atoms and the imidazole N and C atoms of 84°. Phenyl atom H6 is positioned above imidazole atom N1, with an N1—C4—C5—C6 torsion angle of 13.0 (4)° and an H6···N1 distance of 2.58 Å, compared to the sum of the van der Waals radii of 2.75 Å (Bondi, 1964). There is also a close contact between one of the benzyl H atoms and the I atom, with an H4*B*···I1 distance of 3.04 Å, compared to the sum of the van der Waals radii of 3.18 Å. The three-dimensional structure of (1) features an imidazole N···I halogen bond, as shown in Fig. 1. The N2···I1[i] distance [symmetry code: (i) $x − \frac{1}{2}, −y + \frac{1}{2}, −z + 1$] is 2.8765 (2) Å, which is 81% of the sum of the van der Waals radii of 3.53 Å (Bondi, 1964). The halogen bond is almost linear, with a C—I···N angle of 174.42 (9)°.

Linear one-dimensional ribbons of zigzag halogen-bonded molecules of (1) dominate the three-dimensional structure, as shown in Fig. 2. These one-dimensional ribbons run parallel to the *a* axis and are close packed with no other significant intermolecular interactions.

The X-ray structure of (2) also contains a single molecule in the asymmetric unit having a bent shape. The phenyl group is also almost orthogonal to the imidazole group, with a dihedral angle between the planes defined by the phenyl and imidazole rings of 84°. The phenyl ring is not oriented above the imidazole ring; the C6—C5—C4—N1 torsion angle is −52.0 (2)°. The three-dimensional structure has a weak iodo–π interaction involving the pendant phenyl ring of an
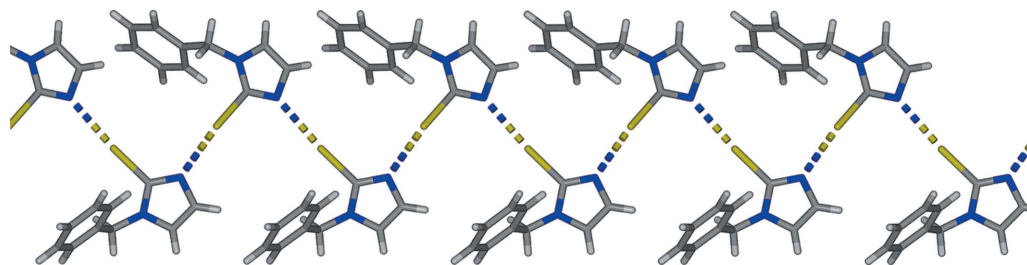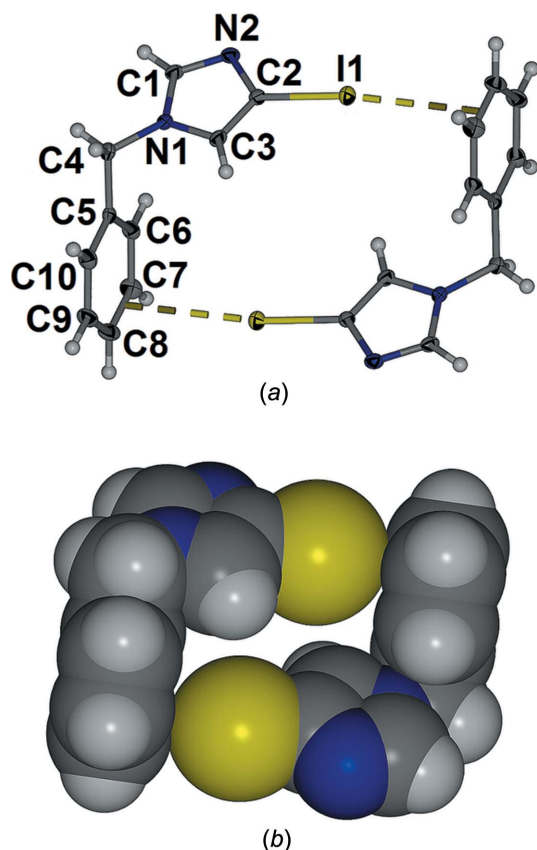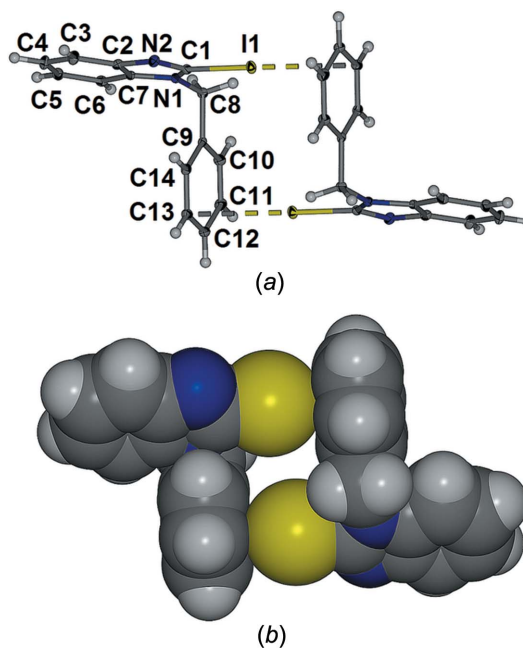

Figure 2
The one-dimensional zigzag halogen-bonded ribbon of molecules in the single-crystal X-ray structure of (1).

Figure 3
The molecular structure of (2), showing (a) the atom labeling and the C—I···π(phenyl) interactions (dashed lines), with displacement ellipsoids drawn at the 50% probability level, and (b) a space-filling model.

adjacent molecule that results in the formation of C—I···π halogen-bonded dimers, as shown in Fig. 3.

In the C—I···π-bonded dimer of (2), the C—I bond is directed towards phenyl atoms C7^{i} and C8^{i} [symmetry code: (i) $-x + 1$, $-y + 1$, $-z + 2$] of an adjacent molecule, with I1···C7^{i} and I1···C8^{i} distances of 3.551 (2) and 3.5534 (2) Å, respectively, both approximately 96% of the sum of the van der

Figure 4
The structure of the C—I···π halogen-bonded dimers formed in the structure of (3), showing (a) the atom labeling and the C—I···π(phenyl) interactions (dashed lines), with displacement ellipsoids drawn at the 50% probability level, and (b) a space-filling model.

Waals radii of 3.68 Å (Bondi, 1964). The C2—I1···C7^{i} and C2—I1···C8^{i} angles are 152.99 (1) and 171.24 (1)°, respectively. The C—I···Cg1^{i} distance is 3.5861 (2) Å (Cg1 is the centroid of the C5–C10 phenyl ring) and the C—I···Cg1^{i} angle is 162.82 (1)°. There are two other close contacts in the three-dimensional structure of (2). One of these is a nonconventional C—H···N hydrogen bond between atom N2 and a benzylic H atom of an adjacent molecule, with an N2···H4B^{ii} [symmetry code: (ii) x, $y - 1$, z] distance of 2.55 Å, which is 93% of the sum of the van der Waals radii of 2.75 Å (Bondi, 1964); the C—H···N angle is 158°. There is a close H···H contact of 2.26 Å between atoms H4A and H7^{iii} [symmetry code: (iii) $-x + \frac{1}{2}$, $y + \frac{1}{2}$, $-z + \frac{3}{2}$] of an adjacent molecule.
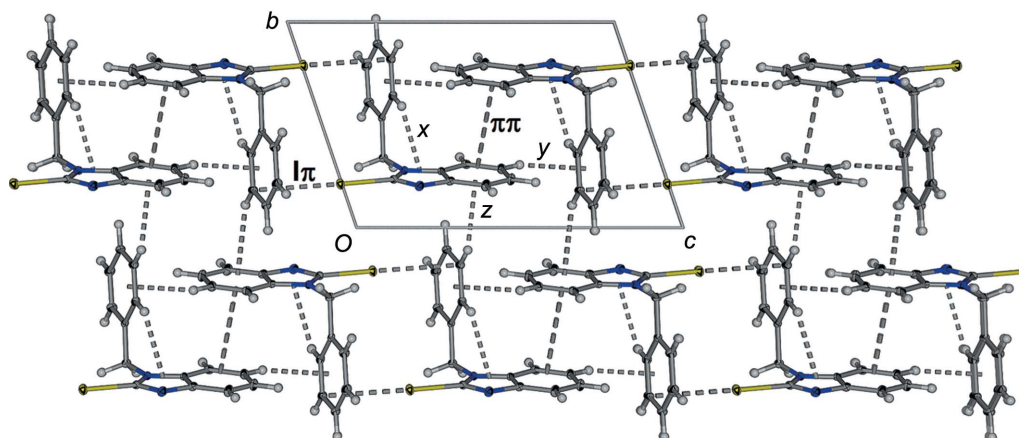
Figure 5
A partial view of the three-dimensional packing of (3), viewed along the a axis. The C—I···π interaction is labeled as Iπ, the C—H···π interactions are labeled as x, y and z, and the π-stacking is labeled as $\pi\pi$.
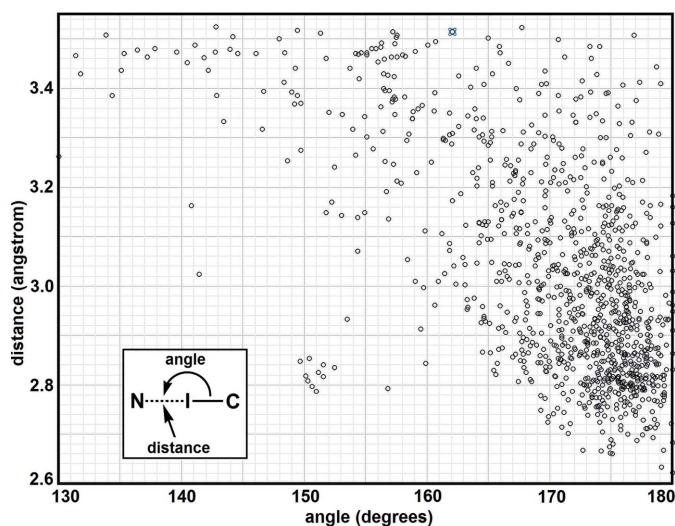
Figure 6
A scatterplot of the N···I distances and C—I···N angles corresponding to all results of a search of the CSD using *Conquest* for C—I···N contacts with an I···N distance less than or equal to 3.53 Å, *i.e.* the sum of the van der Waals radii, and an C—I···N angle between 120 and 180°.

The structure of (3) also contains a single molecule in the asymmetric unit, with a dihedral angle between the imidazole and benzyl rings of 86°. In this structure, phenyl atom H9 is positioned above atom N1, with an N1—C8—C9—C14 torsion angle of -13.4 (2)°. There is also a C—I···π interaction to the phenyl ring of an adjacent molecule, resulting in a C—I···π-bonded molecular dimeric motif similar to that observed in (2) (Fig. 4).

In the C—I···π-bonded dimer of (3), the C—I bond is directed towards phenyl atom C13[i] [symmetry code: (i) $-x + 1$, $-y + 1$, $-z$] of the adjacent molecule, with a C1—I1···C13[i] angle of 178.66 (1)° and an I3···C13[i] distance of 3.3929 (4) Å. This distance is 92% of the sum of the van der Waals radii of 3.68 Å (Bondi, 1964). The C—I···Cg1[i] distance is 3.4562 (4) Å (Cg1 is the centroid of the C9–C14 phenyl ring) and the C—I···Cg1[i] angle is 156.94 (1)°. There is an intramolecular C—H···π interaction since benzyl atom H14 lies above the imidazole ring, with an N1—C8—C9—C14 torsion angle of -13.4 (2)°. This interaction is labeled '*x*' in Fig. 5. The H14···N1 distance is 2.51 Å and the C14—H14···N1 angle is 101°. The H14···Cg2 distance is 2.82 Å (Cg2 is the centroid of the N1/C1/N2/C2/C7 imidazole ring) and the C14—H14···Cg2 angle is 125°.

The three-dimensional packing of (3) involves multiple cohesive interactions, namely two intermolecular C—H···π interactions and two π–π interactions. Benzimidazole atom H5 is involved in a C—H···π interaction with the pendant phenyl ring, labeled '*y*' in Fig. 5; the H5···Cg1[ii] distance is 2.78 Å and the C—H···Cg1[ii] angle is 149° [Cg1 is the centroid of C9–C14 ring; symmetry code: (ii) $-x + 2$, $-y + 1$, $-z + 1$]. Benzyl atom H13 is involved in an interaction with the benzimidazole benzene ring, labeled '*z*' in Fig. 5, with an H13···Cg3[iii] distance of 2.94 Å and a C13—H13···Cg3[iii] angle of 141° [Cg3 is the centroid of the benzimidazole C2–C7 ring; symmetry code: (iii) x, $y + 1$, z]. The benzimidazole groups are

alternately π-stacked (labeled ππ in Fig. 5), with the benzene rings overlaid and slightly offset. The Cg3···Cg3[iv] distance is 4.5536 (6) Å, the perpendicular distance between the benzene rings is 4.3405 Å and the slippage is 1.377 Å [symmetry code: (iv) $-x + 1$, $-y + 1$, $-z + 1$].

In order to place these C—I···N and C—I···π interactions in context, two searches of the Cambridge Structural Database (CSD, Version 5.37; Groom *et al.*, 2016) using *Conquest* (Bruno *et al.*, 2002) were made. The first search, for crystal structures containing C—I···N contacts with I···N distances equal to or less than the sum of the van der Waals radii (3.53 Å), yielded 763 structures with a total of 1082 contacts that met the criteria. Several of these structures corresponded to parallel-displaced π-stacked aromatics, with very short contacts and C—I···N angles less than 90°, which we deemed as significantly different to not include in the analysis. Accordingly, the search was modified to include those structures in which the C—I···N angle was between 120 and 180°, resulting in 752 structures with 1058 distinct interactions that are displayed in the scatterplot of N···I distance *versus* C—I···N angle in Fig. 6. The N···I distance reported here for (1) [2.876 (3) Å] is less than the median (2.973 Å) of the 1058 reported N···I distances and is clearly in the group of shorter C—I···N interactions. The almost linear C—I···N angle is consistent with the majority of the shorter N···I distances which are clustered at C—I···N angles above 165°.

The second search of the CSD using *Conquest* probed C—I···π interactions specifically between an I atom bonded to carbon and a benzene ring as the π-system in which the I···Cg (Cg is the centroid of the benzene ring) distance was less than 3.68 Å (the sum of the van der Waals radii of C and I) and the C—I···π angles were between 120 and 180°. The restrictive angle was chosen to exclude parallel-displaced π-stacked systems. The shortest C—I···Cg distance from the search (3.215 Å) was recorded from a crystal of 2-(2-fluoropyridin-3-yl)-2-(4-iodophenyl)-2*H*-3λ⁵,2λ⁵-[1,3,2]oxazaborolo[5,4,3-*ij*]
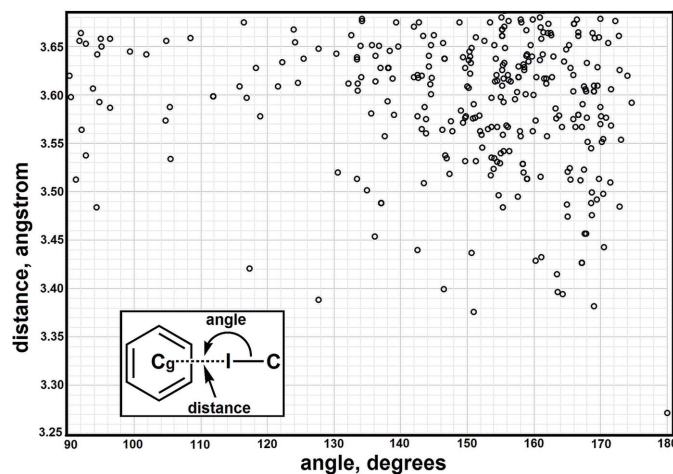
Figure 7
A scatterplot showing the C—I···Cg contacts (Cg is the centroid of the benzene ring) to benzene derivatives, with an I···Cg distance less than or equal to 3.68 Å, *i.e.* the sum of the van der Waals radii, and an C—I···Cg angle between 120 and 180°.
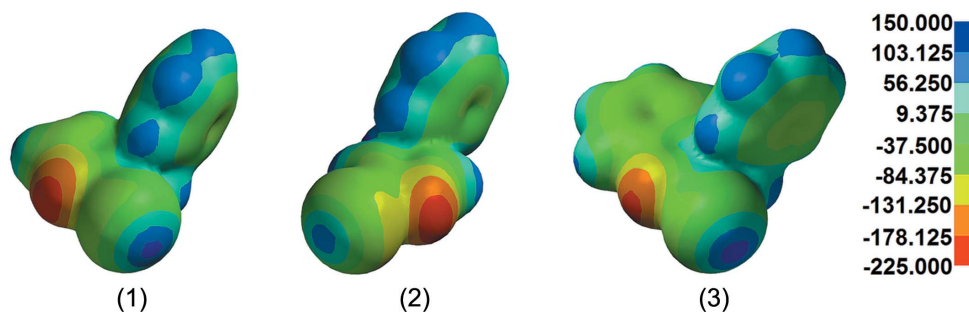
Figure 8
The molecular electrostatic potential maps of compounds (1), (2), and (3), shown on the same scale (right).

quinolone under a pressure of 4.88 GPa at ambient temperature (Wesela-Bauman *et al.*, 2014). In fact, four of the five shortest C—I···*Cg* distances reported correspond to that study. The C—I···*Cg* distance for the same compound at 100 K and under atmospheric pressure is 3.525 Å. Accordingly, the data corresponding to pressurized crystals from that study are not included in the scatterplot of I···*Cg* distances *versus* C—I···*Cg* angles displayed in Fig. 7.

The shortest C—I···*Cg* distance of 3.272 Å in Fig. 7 corresponds to the structure of the *p*-xylene solvate of hexakis(4-iodophenyl)benzene that includes an iodo–π interaction between one of the iodobenzene molecules and the included *p*-xylene solvent molecule (Kobayashi *et al.*, 2005). The next six close contacts have C—I···*Cg* distances between 3.376 and 3.400 Å. The C—I···*Cg* distance of 3.4562 (4) Å reported here for (3) is clearly amongst the shorter C—I···*Cg* distances reported to date.

In order to better understand the halogen-bonding behavior of (1), (2), and (3), the molecular electrostatic potentials of these three compounds were calculated and the plots showing the molecular electrostatic potential surfaces are shown in Fig. 8.

The calculated positive electrostatic potential associated with the positive σ-hole on the I atom of compounds (1), (2), and (3) were determined to be 123, 81, and 129 kJ mol^{-1}, respectively. These modest values associated with the positive σ-hole are considerably lower than the values reported for the better known halogen-bond donors. For example, iodopentafluorobenzene has a calculated positive electrostatic potential associated with the σ-hole on the I atom of 166 kJ mol^{-1} (Aakeröy *et al.*, 2014). The positive electrostatic potential associated with the σ-hole on the I atom of 1,3,5-triiodo-2,4,6-trinitrobenzene has recently been reported as 213 kJ mol^{-1}, which is the most positive value calculated to date (Goud *et al.*, 2016). Nevertheless, the 2-iodoimidazole derivatives are distinctly better halogen-bond donors than iodobenzene, with a calculated electrostatic potential of 103 kJ mol^{-1} (Aakeröy *et al.*, 2014), while the 4-iodoimidazole derivative is a poorer halogen-bond acceptor than iodobenzene. The negative electrostatic potential on the unsubstituted N atom of compounds (1), (2), and (3) are −204, −210, and −193 kJ mol^{-1}, respectively. These values are similar to the values reported for a series of *N*-substituted imidazole derivatives (Aakeröy *et al.*, 2016). Thus, while the relatively weak halogen-bonding

interaction of (2) can be ascribed to the low positive electrostatic potential on the I atom, rationalizing the other two results is difficult. The conundrum is that compounds (1) and (3) have similar halogen-bond-donor properties and similar halogen-bond-acceptor properties on the unsubstituted imidazole N atom, yet form different types of halogen bonds (C—I···N *versus* C—I···π).

In conclusion, we have demonstrated that 2-iodoimidazoles are effective halogen-bond donors and acceptors and may form C—I···N or C—I···π halogen bonds but we are, as yet, unable to rationalize the factors that control the type of halogen bonding. In our future work, we plan to explore intra- and intermolecular C—I···π interactions.

Acknowledgements

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supporting information

C—I⋯N and C—I⋯π halogen bonding in the structures of 1-benzyliodo-imidazole derivatives

Chideraa I. Nwachukwu, Nathan P. Bowling and Eric Bosch

Computing details

For all structures, data collection: *SMART* (Bruker, 2014); cell refinement: *SMART* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED* (Barbour, 2001).

1-Benzyl-2-iodo-1*H*-imidazole (1)

Crystal data

$C_{10}H_9IN_2$	$D_x = 1.858$ Mg m^{-3}
$M_r = 284.09$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 7864 reflections
$a = 8.7561$ (5) Å	$\theta = 2.8–27.1°$
$b = 9.0016$ (5) Å	$\mu = 3.11$ mm^{-1}
$c = 12.8869$ (7) Å	$T = 100$ K
$V = 1015.73$ (10) Å^3	Irregular, colourless
$Z = 4$	$0.30 \times 0.20 \times 0.05$ mm
$F(000) = 544$	

Data collection

Bruker APEXII CCD diffractometer	13262 measured reflections
Radiation source: fine-focus sealed tube	2228 independent reflections
Graphite monochromator	2202 reflections with $I > 2\sigma(I)$
Detector resolution: 8.3660 pixels mm^{-1}	$R_{int} = 0.030$
phi and ω scans	$\theta_{max} = 27.1°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$h = -11 \rightarrow 11$
	$k = -11 \rightarrow 11$
	$l = -16 \rightarrow 16$
$T_{min} = 0.622$, $T_{max} = 0.746$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0131P)^2 + 0.0966P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.013$	
$wR(F^2) = 0.030$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
2228 reflections	$\Delta\rho_{min} = -0.27$ e Å^{-3}
118 parameters	Absolute structure: Flack x determined using 913 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
0 restraints	
Hydrogen site location: inferred from neighbouring sites	Absolute structure parameter: −0.002 (13)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.23697 (2)	0.28234 (2)	0.52915 (2)	0.01308 (5)
N1	0.1137 (3)	0.4336 (3)	0.72457 (18)	0.0140 (5)
C1	0.0779 (3)	0.3510 (3)	0.6399 (2)	0.0126 (6)
N2	−0.0686 (3)	0.3169 (3)	0.63687 (19)	0.0153 (5)
C2	−0.1294 (3)	0.3814 (3)	0.7256 (2)	0.0175 (6)
H1	−0.2337	0.3759	0.7456	0.021*
C3	−0.0203 (3)	0.4526 (3)	0.7792 (2)	0.0173 (6)
H9	−0.0329	0.5057	0.8423	0.021*
C4	0.2632 (4)	0.4913 (3)	0.7544 (2)	0.0163 (6)
H7	0.2484	0.5859	0.7923	0.020*
H8	0.3218	0.5138	0.6906	0.020*
C5	0.3573 (3)	0.3881 (3)	0.8214 (2)	0.0145 (6)
C6	0.3217 (3)	0.2395 (3)	0.8364 (2)	0.0165 (6)
H3	0.2345	0.1980	0.8035	0.020*
C7	0.4136 (3)	0.1504 (4)	0.8995 (2)	0.0210 (7)
H4	0.3885	0.0487	0.9094	0.025*
C8	0.5407 (3)	0.2094 (4)	0.9477 (2)	0.0215 (7)
H2	0.6027	0.1487	0.9909	0.026*
C9	0.5776 (4)	0.3587 (4)	0.9327 (2)	0.0222 (7)
H5	0.6647	0.4001	0.9658	0.027*
C10	0.4869 (3)	0.4463 (3)	0.8693 (2)	0.0177 (6)
H6	0.5134	0.5474	0.8583	0.021*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01264 (8)	0.01415 (9)	0.01244 (8)	0.00140 (7)	0.00028 (7)	−0.00020 (6)
N1	0.0139 (12)	0.0132 (12)	0.0150 (12)	0.0009 (10)	−0.0017 (10)	−0.0015 (10)
C1	0.0138 (14)	0.0102 (13)	0.0138 (14)	0.0027 (11)	−0.0002 (11)	0.0008 (11)
N2	0.0134 (11)	0.0163 (14)	0.0161 (12)	0.0017 (9)	−0.0001 (9)	0.0000 (9)
C2	0.0153 (14)	0.0183 (16)	0.0189 (15)	0.0027 (12)	0.0024 (12)	−0.0005 (12)
C3	0.0206 (16)	0.0178 (15)	0.0135 (14)	0.0043 (13)	0.0023 (13)	−0.0010 (12)
C4	0.0169 (14)	0.0147 (13)	0.0172 (12)	−0.0036 (12)	−0.0032 (15)	−0.0006 (10)
C5	0.0142 (14)	0.0182 (15)	0.0110 (14)	0.0018 (12)	0.0021 (11)	−0.0028 (11)
C6	0.0148 (13)	0.0173 (16)	0.0174 (13)	−0.0015 (11)	−0.0003 (11)	−0.0018 (12)
C7	0.0222 (16)	0.0204 (15)	0.0203 (15)	0.0022 (13)	0.0067 (13)	0.0026 (13)
C8	0.0211 (14)	0.0277 (17)	0.0156 (14)	0.0087 (15)	−0.0008 (11)	0.0024 (14)
C9	0.0171 (15)	0.0285 (18)	0.0210 (16)	0.0039 (14)	−0.0034 (12)	−0.0039 (14)
C10	0.0169 (15)	0.0168 (15)	0.0195 (15)	−0.0010 (12)	0.0007 (13)	−0.0037 (13)

Geometric parameters (Å, º)

I1—C1	2.088 (3)	C5—C6	1.387 (4)
N1—C1	1.357 (4)	C5—C10	1.394 (4)
N1—C3	1.379 (3)	C6—C7	1.397 (4)
N1—C4	1.461 (4)	C6—H3	0.9500
C1—N2	1.319 (3)	C7—C8	1.381 (4)
N2—C2	1.389 (4)	C7—H4	0.9500
C2—C3	1.341 (4)	C8—C9	1.395 (5)
C2—H1	0.9500	C8—H2	0.9500
C3—H9	0.9500	C9—C10	1.386 (4)
C4—C5	1.512 (4)	C9—H5	0.9500
C4—H7	0.9900	C10—H6	0.9500
C4—H8	0.9900		
C1—N1—C3	106.4 (2)	C6—C5—C10	118.9 (3)
C1—N1—C4	127.8 (2)	C6—C5—C4	123.4 (3)
C3—N1—C4	125.8 (2)	C10—C5—C4	117.7 (3)
N2—C1—N1	112.1 (2)	C5—C6—C7	120.4 (3)
N2—C1—I1	124.0 (2)	C5—C6—H3	119.8
N1—C1—I1	123.9 (2)	C7—C6—H3	119.8
C1—N2—C2	104.5 (2)	C8—C7—C6	120.3 (3)
C3—C2—N2	110.5 (3)	C8—C7—H4	119.8
C3—C2—H1	124.7	C6—C7—H4	119.8
N2—C2—H1	124.7	C7—C8—C9	119.7 (3)
C2—C3—N1	106.5 (3)	C7—C8—H2	120.2
C2—C3—H9	126.8	C9—C8—H2	120.2
N1—C3—H9	126.8	C10—C9—C8	119.8 (3)
N1—C4—C5	114.8 (2)	C10—C9—H5	120.1
N1—C4—H7	108.6	C8—C9—H5	120.1
C5—C4—H7	108.6	C9—C10—C5	120.9 (3)
N1—C4—H8	108.6	C9—C10—H6	119.5
C5—C4—H8	108.6	C5—C10—H6	119.5
H7—C4—H8	107.5		
C3—N1—C1—N2	0.2 (3)	C3—N1—C4—C5	90.2 (3)
C4—N1—C1—N2	179.7 (2)	N1—C4—C5—C6	13.0 (4)
C3—N1—C1—I1	−178.7 (2)	N1—C4—C5—C10	−167.7 (2)
C4—N1—C1—I1	0.9 (4)	C10—C5—C6—C7	0.8 (4)
N1—C1—N2—C2	−0.3 (3)	C4—C5—C6—C7	−179.9 (3)
I1—C1—N2—C2	178.5 (2)	C5—C6—C7—C8	0.0 (4)
C1—N2—C2—C3	0.3 (3)	C6—C7—C8—C9	−0.3 (4)
N2—C2—C3—N1	−0.2 (3)	C7—C8—C9—C10	−0.2 (4)
C1—N1—C3—C2	0.1 (3)	C8—C9—C10—C5	1.1 (4)
C4—N1—C3—C2	−179.5 (3)	C6—C5—C10—C9	−1.4 (4)
C1—N1—C4—C5	−89.3 (3)	C4—C5—C10—C9	179.3 (3)

1-Benzyl-4-iodo-1*H*-benzimidazole (2)

Crystal data

$C_{10}H_9IN_2$	$F(000) = 544$
$M_r = 284.09$	$D_x = 1.878$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.4574$ (5) Å	Cell parameters from 7481 reflections
$b = 6.1526$ (3) Å	$\theta = 2.5–27.1°$
$c = 19.4261$ (10) Å	$\mu = 3.14$ mm^{-1}
$\beta = 96.362$ (1)°	$T = 100$ K
$V = 1004.61$ (9) Å^3	Cut irregular cube, colourless
$Z = 4$	$0.22 \times 0.22 \times 0.22$ mm

Data collection

Bruker APEXII CCD diffractometer	12374 measured reflections
Radiation source: fine-focus sealed tube	2207 independent reflections
Graphite monochromator	2114 reflections with $I > 2\sigma(I)$
Detector resolution: 8.3660 pixels mm^{-1}	$R_{int} = 0.021$
phi and ω scans	$\theta_{max} = 27.1°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$h = -10\rightarrow10$
	$k = -7\rightarrow7$
$T_{min} = 0.594$, $T_{max} = 0.746$	$l = -24\rightarrow24$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.016$	$w = 1/[\sigma^2(F_o^2) + (0.0133P)^2 + 0.8316P]$
$wR(F^2) = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} = 0.002$
2207 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.52$ e Å^{-3}
0 restraints	

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 (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
I1	0.78435 (2)	0.28882 (2)	0.99037 (2)	0.02415 (5)
N1	0.62017 (18)	0.7607 (3)	0.84311 (8)	0.0184 (3)
C1	0.6885 (2)	0.6133 (3)	0.80429 (9)	0.0193 (4)
H1	0.6911	0.6269	0.7557	0.023*
N2	0.75130 (18)	0.4480 (3)	0.84125 (8)	0.0202 (3)
C2	0.7195 (2)	0.4950 (3)	0.90773 (9)	0.0176 (4)
C3	0.6390 (2)	0.6861 (3)	0.91019 (9)	0.0202 (4)
H3	0.6035	0.7533	0.9497	0.024*
C4	0.5408 (2)	0.9614 (3)	0.81736 (10)	0.0234 (4)
H4A	0.5420	0.9692	0.7665	0.028*

H4B	0.6011	1.0876	0.8381	0.028*
C5	0.3709 (2)	0.9758 (3)	0.83403 (9)	0.0180 (4)
C6	0.2651 (2)	0.8056 (3)	0.81699 (10)	0.0212 (4)
H6	0.3005	0.6781	0.7958	0.025*
C7	0.1081 (2)	0.8218 (3)	0.83096 (10)	0.0256 (4)
H7	0.0365	0.7048	0.8197	0.031*
C8	0.0554 (2)	1.0088 (4)	0.86130 (10)	0.0265 (4)
H8	−0.0523	1.0201	0.8705	0.032*
C9	0.1594 (3)	1.1779 (3)	0.87815 (11)	0.0277 (4)
H9	0.1231	1.3058	0.8988	0.033*
C10	0.3176 (2)	1.1619 (3)	0.86495 (10)	0.0240 (4)
H10	0.3891	1.2783	0.8771	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02821 (8)	0.02566 (8)	0.01895 (7)	0.00504 (5)	0.00421 (5)	0.00451 (5)
N1	0.0185 (8)	0.0183 (8)	0.0193 (8)	0.0004 (6)	0.0055 (6)	0.0031 (6)
C1	0.0177 (9)	0.0255 (10)	0.0152 (8)	0.0006 (7)	0.0038 (7)	−0.0016 (7)
N2	0.0198 (8)	0.0235 (8)	0.0177 (7)	0.0025 (6)	0.0045 (6)	−0.0027 (6)
C2	0.0171 (8)	0.0191 (9)	0.0167 (8)	0.0005 (7)	0.0027 (7)	0.0004 (7)
C3	0.0248 (10)	0.0203 (10)	0.0167 (9)	0.0003 (7)	0.0075 (7)	0.0000 (7)
C4	0.0248 (10)	0.0186 (9)	0.0281 (10)	0.0021 (8)	0.0089 (8)	0.0080 (8)
C5	0.0211 (9)	0.0178 (9)	0.0151 (8)	0.0028 (7)	0.0022 (7)	0.0043 (7)
C6	0.0259 (10)	0.0184 (9)	0.0190 (9)	0.0042 (7)	0.0009 (7)	−0.0028 (7)
C7	0.0212 (10)	0.0305 (12)	0.0236 (10)	−0.0015 (8)	−0.0045 (8)	−0.0048 (8)
C8	0.0195 (9)	0.0380 (12)	0.0216 (9)	0.0078 (8)	0.0004 (7)	−0.0019 (8)
C9	0.0314 (11)	0.0263 (11)	0.0257 (10)	0.0106 (9)	0.0050 (8)	−0.0037 (8)
C10	0.0279 (10)	0.0185 (10)	0.0254 (10)	0.0007 (8)	0.0015 (8)	−0.0010 (8)

Geometric parameters (Å, º)

I1—C2	2.0717 (18)	C5—C10	1.391 (3)
N1—C1	1.349 (2)	C5—C6	1.393 (3)
N1—C3	1.374 (2)	C6—C7	1.388 (3)
N1—C4	1.467 (2)	C6—H6	0.9500
C1—N2	1.322 (2)	C7—C8	1.388 (3)
C1—H1	0.9500	C7—H7	0.9500
N2—C2	1.379 (2)	C8—C9	1.378 (3)
C2—C3	1.362 (3)	C8—H8	0.9500
C3—H3	0.9500	C9—C10	1.394 (3)
C4—C5	1.510 (3)	C9—H9	0.9500
C4—H4A	0.9900	C10—H10	0.9500
C4—H4B	0.9900		
C1—N1—C3	107.09 (15)	C10—C5—C6	119.40 (17)
C1—N1—C4	125.67 (16)	C10—C5—C4	120.18 (18)
C3—N1—C4	127.24 (16)	C6—C5—C4	120.39 (17)

N2—C1—N1	112.62 (16)	C7—C6—C5	120.18 (18)
N2—C1—H1	123.7	C7—C6—H6	119.9
N1—C1—H1	123.7	C5—C6—H6	119.9
C1—N2—C2	103.82 (15)	C8—C7—C6	120.08 (19)
C3—C2—N2	111.35 (16)	C8—C7—H7	120.0
C3—C2—I1	126.28 (13)	C6—C7—H7	120.0
N2—C2—I1	122.34 (13)	C9—C8—C7	120.02 (19)
C2—C3—N1	105.11 (16)	C9—C8—H8	120.0
C2—C3—H3	127.4	C7—C8—H8	120.0
N1—C3—H3	127.4	C8—C9—C10	120.24 (19)
N1—C4—C5	112.76 (15)	C8—C9—H9	119.9
N1—C4—H4A	109.0	C10—C9—H9	119.9
C5—C4—H4A	109.0	C5—C10—C9	120.08 (19)
N1—C4—H4B	109.0	C5—C10—H10	120.0
C5—C4—H4B	109.0	C9—C10—H10	120.0
H4A—C4—H4B	107.8		
C3—N1—C1—N2	−0.3 (2)	N1—C4—C5—C10	129.69 (19)
C4—N1—C1—N2	179.94 (17)	N1—C4—C5—C6	−52.0 (2)
N1—C1—N2—C2	0.3 (2)	C10—C5—C6—C7	−0.2 (3)
C1—N2—C2—C3	−0.1 (2)	C4—C5—C6—C7	−178.49 (18)
C1—N2—C2—I1	178.38 (13)	C5—C6—C7—C8	0.7 (3)
N2—C2—C3—N1	0.0 (2)	C6—C7—C8—C9	−0.6 (3)
I1—C2—C3—N1	−178.47 (13)	C7—C8—C9—C10	−0.1 (3)
C1—N1—C3—C2	0.2 (2)	C6—C5—C10—C9	−0.5 (3)
C4—N1—C3—C2	179.96 (17)	C4—C5—C10—C9	177.82 (18)
C1—N1—C4—C5	123.20 (19)	C8—C9—C10—C5	0.7 (3)
C3—N1—C4—C5	−56.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C4—H4B⋯N2^i	0.99	2.55	3.488 (3)	158
C4—H4B⋯N2^i	0.99	2.55	3.488 (3)	158
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Symmetry code: (i) x, $y+1$, z.

1-Benzyl-2-iodo-1*H*-benzimidazole (3)

Crystal data

$C_{14}H_{11}IN_2$
$M_r = 334.15$
Triclinic, $P\overline{1}$
$a = 6.4606$ (8) Å
$b = 8.2346$ (10) Å
$c = 12.3451$ (14) Å
$\alpha = 108.064$ (1)°
$\beta = 94.174$ (2)°

$\gamma = 95.366$ (2)°
$V = 618.05$ (13) Å³
$Z = 2$
$F(000) = 324$
$D_x = 1.796$ Mg m⁻³
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6682 reflections
$\theta = 2.6–27.3$°

$\mu = 2.57$ mm^{-1}
$T = 100$ K

Cut irregular cube, colourless
$0.20 \times 0.20 \times 0.20$ mm

Data collection

Bruker APEXII CCD diffractometer	8079 measured reflections
Radiation source: fine-focus sealed tube	2777 independent reflections
Graphite monochromator	2725 reflections with $I > 2\sigma(I)$
Detector resolution: 8.3660 pixels mm^{-1}	$R_{int} = 0.016$
phi and ω scans	$\theta_{max} = 27.3°$, $\theta_{min} = 1.8°$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$h = -8 \rightarrow 8$
	$k = -10 \rightarrow 10$
$T_{min} = 0.588$, $T_{max} = 0.746$	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.015$	H-atom parameters constrained
$wR(F^2) = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 0.3329P]$
$S = 1.09$	where $P = (F_o^2 + 2F_c^2)/3$
2777 reflections	$(\Delta/\sigma)_{max} < 0.001$
154 parameters	$\Delta\rho_{max} = 0.74$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.35$ e Å^{-3}

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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
I1	0.36505 (2)	0.21176 (2)	−0.00445 (2)	0.01647 (5)
N1	0.6779 (2)	0.27787 (17)	0.20512 (12)	0.0120 (3)
C1	0.4707 (3)	0.2345 (2)	0.16333 (14)	0.0128 (3)
N2	0.3471 (2)	0.20232 (18)	0.23569 (12)	0.0150 (3)
C2	0.4817 (3)	0.2263 (2)	0.33480 (14)	0.0139 (3)
C3	0.4394 (3)	0.2054 (2)	0.43956 (15)	0.0182 (3)
H3	0.3012	0.1724	0.4531	0.022*
C4	0.6071 (3)	0.2349 (2)	0.52297 (15)	0.0194 (4)
H4	0.5828	0.2201	0.5945	0.023*
C5	0.8118 (3)	0.2859 (2)	0.50456 (15)	0.0175 (3)
H5	0.9221	0.3057	0.5641	0.021*
C6	0.8566 (3)	0.3081 (2)	0.40127 (15)	0.0151 (3)
H6	0.9943	0.3438	0.3885	0.018*
C7	0.6875 (3)	0.2749 (2)	0.31748 (14)	0.0122 (3)
C8	0.8525 (3)	0.3389 (2)	0.15353 (14)	0.0132 (3)
H8B	0.8223	0.2938	0.0691	0.016*
H8A	0.9799	0.2929	0.1749	0.016*
C9	0.8940 (3)	0.5343 (2)	0.19092 (13)	0.0117 (3)

C10	1.0811 (3)	0.6095 (2)	0.16685 (15)	0.0158 (3)
H10	1.1789	0.5383	0.1290	0.019*
C11	1.1250 (3)	0.7877 (2)	0.19790 (15)	0.0177 (3)
H11	1.2523	0.8376	0.1811	0.021*
C12	0.9832 (3)	0.8928 (2)	0.25341 (15)	0.0160 (3)
H12	1.0129	1.0144	0.2742	0.019*
C13	0.7972 (3)	0.8192 (2)	0.27853 (14)	0.0150 (3)
H13	0.7006	0.8907	0.3173	0.018*
C14	0.7526 (3)	0.6401 (2)	0.24673 (14)	0.0136 (3)
H14	0.6250	0.5904	0.2633	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01853 (7)	0.01995 (7)	0.01172 (6)	0.00853 (4)	0.00073 (4)	0.00460 (4)
N1	0.0124 (6)	0.0118 (6)	0.0118 (6)	0.0009 (5)	0.0018 (5)	0.0038 (5)
C1	0.0145 (8)	0.0118 (7)	0.0120 (7)	0.0031 (6)	0.0003 (6)	0.0036 (6)
N2	0.0129 (7)	0.0168 (7)	0.0161 (7)	0.0012 (5)	0.0005 (5)	0.0069 (6)
C2	0.0138 (8)	0.0130 (7)	0.0157 (8)	0.0018 (6)	0.0016 (6)	0.0058 (6)
C3	0.0155 (8)	0.0236 (9)	0.0182 (8)	0.0018 (7)	0.0050 (7)	0.0099 (7)
C4	0.0229 (9)	0.0238 (9)	0.0144 (8)	0.0035 (7)	0.0036 (7)	0.0098 (7)
C5	0.0193 (9)	0.0179 (8)	0.0144 (8)	0.0025 (7)	−0.0026 (7)	0.0048 (6)
C6	0.0133 (8)	0.0136 (7)	0.0170 (8)	0.0005 (6)	0.0001 (6)	0.0038 (6)
C7	0.0158 (8)	0.0099 (7)	0.0113 (7)	0.0021 (6)	0.0025 (6)	0.0035 (6)
C8	0.0121 (7)	0.0135 (7)	0.0148 (8)	0.0016 (6)	0.0046 (6)	0.0049 (6)
C9	0.0130 (7)	0.0128 (7)	0.0102 (7)	0.0022 (6)	0.0003 (6)	0.0051 (6)
C10	0.0142 (8)	0.0165 (8)	0.0174 (8)	0.0040 (6)	0.0051 (6)	0.0049 (6)
C11	0.0155 (8)	0.0190 (8)	0.0194 (8)	−0.0008 (6)	0.0040 (7)	0.0078 (7)
C12	0.0199 (8)	0.0129 (7)	0.0151 (8)	0.0010 (6)	0.0011 (6)	0.0048 (6)
C13	0.0161 (8)	0.0142 (8)	0.0150 (8)	0.0045 (6)	0.0028 (6)	0.0043 (6)
C14	0.0122 (7)	0.0159 (8)	0.0141 (8)	0.0021 (6)	0.0029 (6)	0.0063 (6)

Geometric parameters (Å, º)

I1—C1	2.0787 (16)	C6—H6	0.9500
N1—C1	1.372 (2)	C8—C9	1.522 (2)
N1—C7	1.392 (2)	C8—H8B	0.9900
N1—C8	1.459 (2)	C8—H8A	0.9900
C1—N2	1.310 (2)	C9—C14	1.392 (2)
N2—C2	1.398 (2)	C9—C10	1.399 (2)
C2—C3	1.399 (2)	C10—C11	1.392 (2)
C2—C7	1.403 (2)	C10—H10	0.9500
C3—C4	1.388 (3)	C11—C12	1.389 (2)
C3—H3	0.9500	C11—H11	0.9500
C4—C5	1.406 (3)	C12—C13	1.394 (2)
C4—H4	0.9500	C12—H12	0.9500
C5—C6	1.390 (2)	C13—C14	1.399 (2)
C5—H5	0.9500	C13—H13	0.9500

C6—C7	1.393 (2)	C14—H14	0.9500
C1—N1—C7	105.30 (13)	N1—C8—C9	112.67 (13)
C1—N1—C8	129.42 (14)	N1—C8—H8B	109.1
C7—N1—C8	124.77 (14)	C9—C8—H8B	109.1
N2—C1—N1	114.90 (14)	N1—C8—H8A	109.1
N2—C1—I1	122.95 (12)	C9—C8—H8A	109.1
N1—C1—I1	122.10 (12)	H8B—C8—H8A	107.8
C1—N2—C2	103.99 (14)	C14—C9—C10	119.12 (15)
N2—C2—C3	130.02 (16)	C14—C9—C8	122.54 (14)
N2—C2—C7	110.06 (14)	C10—C9—C8	118.33 (14)
C3—C2—C7	119.90 (16)	C11—C10—C9	120.50 (16)
C4—C3—C2	117.39 (16)	C11—C10—H10	119.8
C4—C3—H3	121.3	C9—C10—H10	119.8
C2—C3—H3	121.3	C12—C11—C10	120.19 (16)
C3—C4—C5	121.86 (16)	C12—C11—H11	119.9
C3—C4—H4	119.1	C10—C11—H11	119.9
C5—C4—H4	119.1	C11—C12—C13	119.71 (15)
C6—C5—C4	121.53 (16)	C11—C12—H12	120.1
C6—C5—H5	119.2	C13—C12—H12	120.1
C4—C5—H5	119.2	C12—C13—C14	120.09 (16)
C5—C6—C7	116.04 (16)	C12—C13—H13	120.0
C5—C6—H6	122.0	C14—C13—H13	120.0
C7—C6—H6	122.0	C9—C14—C13	120.39 (15)
N1—C7—C6	131.00 (15)	C9—C14—H14	119.8
N1—C7—C2	105.74 (14)	C13—C14—H14	119.8
C6—C7—C2	123.26 (15)		

C7—N1—C1—N2	−0.68 (19)	C5—C6—C7—C2	1.7 (2)
C8—N1—C1—N2	−172.65 (15)	N2—C2—C7—N1	−0.90 (18)
C7—N1—C1—I1	−178.20 (11)	C3—C2—C7—N1	177.77 (15)
C8—N1—C1—I1	9.8 (2)	N2—C2—C7—C6	179.92 (15)
N1—C1—N2—C2	0.12 (19)	C3—C2—C7—C6	−1.4 (3)
I1—C1—N2—C2	177.62 (11)	C1—N1—C8—C9	93.38 (19)
C1—N2—C2—C3	−178.00 (18)	C7—N1—C8—C9	−77.17 (19)
C1—N2—C2—C7	0.49 (18)	N1—C8—C9—C14	−13.4 (2)
N2—C2—C3—C4	178.48 (17)	N1—C8—C9—C10	167.25 (14)
C7—C2—C3—C4	0.1 (3)	C14—C9—C10—C11	−0.2 (2)
C2—C3—C4—C5	0.8 (3)	C8—C9—C10—C11	179.10 (15)
C3—C4—C5—C6	−0.5 (3)	C9—C10—C11—C12	0.1 (3)
C4—C5—C6—C7	−0.7 (3)	C10—C11—C12—C13	0.4 (3)
C1—N1—C7—C6	−179.98 (17)	C11—C12—C13—C14	−0.8 (3)
C8—N1—C7—C6	−7.5 (3)	C10—C9—C14—C13	−0.1 (2)
C1—N1—C7—C2	0.92 (17)	C8—C9—C14—C13	−179.45 (15)
C8—N1—C7—C2	173.37 (14)	C12—C13—C14—C9	0.6 (3)
C5—C6—C7—N1	−177.29 (16)		