Structural analysis of 2-iodobenzamide and 2-iodo-*N*-phenylbenzamide

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The title compounds, 2-iodobenzamide, C_7H_6INO (I), and 2-iodo-*N*-phenylbenzamide, $C_{13}H_{10}INO$ (II), were both synthesized from 2-iodobenzoic acid. In the crystal structure of (I), N—H···O and hydrogen bonds form two sets of closed rings, generating dimers and tetramers. These combine with C—I···π(ring) halogen bonds to form sheets of molecules in the *bc* plane. For (II), N—H···O hydrogen bonds form chains along the *a*-axis direction, while inversion-related C—I···π(ring) contacts supported by C—H···π(ring) interactions generate sheets of molecules along the *ab* diagonal.

1. Chemical context

Aromatic amides can be found in a wide range of aromatic molecules and they also serve as intermediates in the production of many pharmaceutical compounds (Suchetan *et al.*, 2016). Aromatic amides and *N*-aryl amides display a wide spectrum of pharmacological properties and are used as antibacterial (Ragavan *et al.*, 2010), analgesic (Starmer *et al.*, 1971), antiviral (Hu *et al.*, 2008), anti-inflammatory (Kalgutkar *et al.*, 2000) and anti-cancer (Pradidphol *et al.*, 2012) agents. Furthermore, *N*-aryl amides are known to act as anti-tumor agents against a broad spectrum of human tumors (Abdou *et al.*, 2004). In view of their potential importance, the title compounds (I) and (II) were synthesized and we report herein a comparison of their structures.
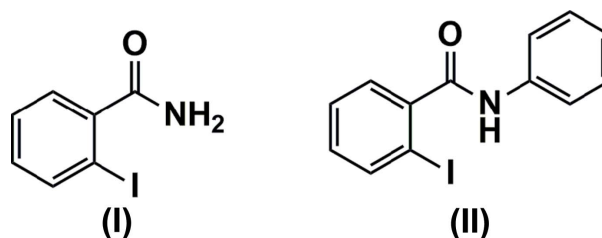
2. Structural commentary

Both compounds (I) and (II) crystallize with one molecule in the asymmetric unit ($Z' = 1$). The molecular structures of the molecules are shown in Figs. 1 and 2, respectively. In (I) the aromatic ring is inclined to the O1/C1/N1 plane of the amide by 44.37 (1)° whereas in (II) the two aromatic rings are almost
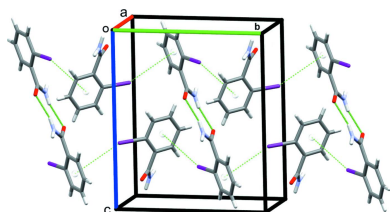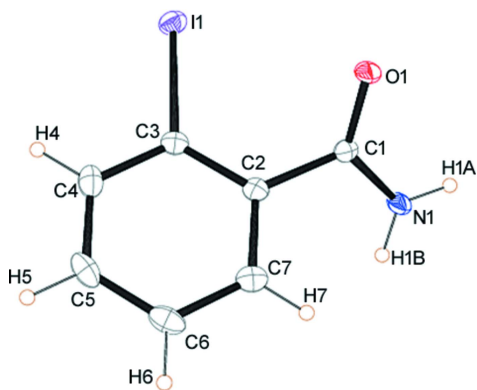
Figure 1
The molecular structure of (I) showing the atom numbering with ellipsoids drawn at the 50% probability level.
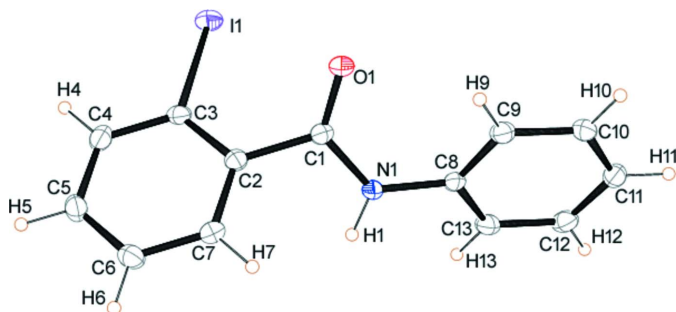

Figure 2
The molecular structure of (II) showing the atom numbering with ellipsoids drawn at the 50% probability level.

orthogonal with an angle of 79.84 (6)° between them. The iodobenzene ring plane is inclined to the O1/C1/N1 amide plane by 52.01 (1)°, somewhat similar to the inclination found for (I), while the phenyl ring of the amide is inclined by 28.45 (5)° to this plane.

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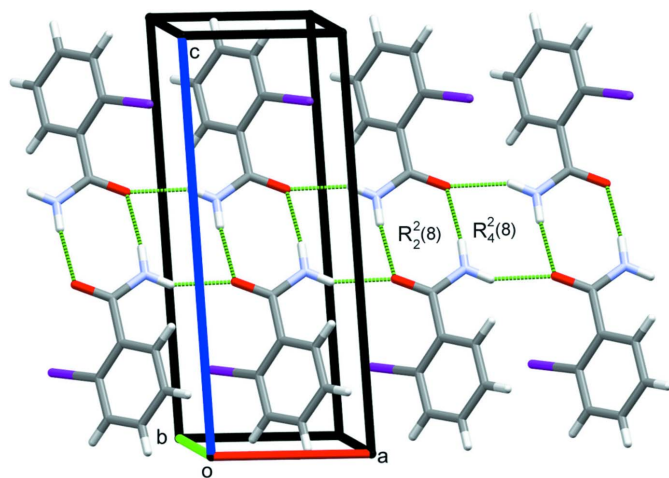Hydrogen-bond geometry (Å, °) for (I).

$Cg1$ is the centroid of the C2–C7 phenyl ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$A\cdots$O1^i	0.86	2.11	2.951 (2)	164
N1—H1$B\cdots$O1^{ii}	0.86	2.05	2.843 (2)	154
C3—I1$\cdots Cg1^{iii}$	2.11 (1)	3.99 (1)	5.877 (2)	148 (1)

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

$Cg2$ is the centroid of the C8–C13 benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1^i	0.88	2.15	2.942 (2)	150
C3—I1$\cdots Cg2^{ii}$	2.10 (1)	3.83 (1)	5.816 (2)	156 (1)
C6—H6$\cdots Cg2^{iii}$	0.95	2.81	3.627 (2)	144

Symmetry codes: (i) $x + 1, y, z$; (ii) $-x, -y, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$.

3. Supramolecular features

In the crystal structure of compound (I), strong classical N1—H1$A\cdots$O1 and N1—H1$B\cdots$O1 hydrogen bonds, Table 1, arrange the molecules in two linked sets of closed rings, forming both dimers with an $R_2^2(8)$ graph-set motif and tetramers that enclose $R_4^2(8)$ rings (Etter *et al.*, 1990). These contacts form chains of molecules along the *a*-axis direction (Fig. 3). In addition, C3—I1$\cdots Cg1$ halogen bonds, Table 1, combine with the previously mentioned inversion dimers to generate sheets of molecules in the *bc* plane (Fig. 4).

For compound (II), the absence of a second H atom on the N1 amine nitrogen atom limits the formation of classical hydrogen bonds to N1—H1$\cdots$O1 contacts that generate $C(4)$ molecular chains along the *a*-axis direction (Fig. 5, Table 2). Additional weak inversion-related C3—I1$\cdots Cg2$ interactions (Table 2), in this instance also supported by C6—H6$\cdots Cg2$ contacts that also lie about an inversion centre, form sheets of molecules along the *ab* diagonal (Fig. 6, Table 2).

Figure 3
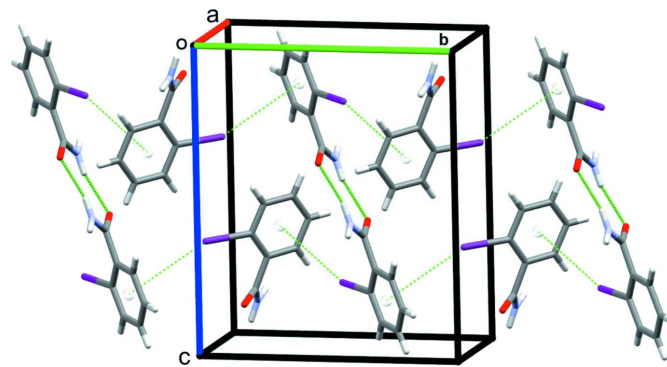Chains of molecules of (I) along the *a*-axis direction, showing the dimers and tetramers formed by N—H$\cdots$O hydrogen bonds.

Figure 4
N—H$\cdots$O and C—I$\cdots\pi$(ring) contacts forming sheets of molecules of (I) in the *bc* plane.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	C_7H_6INO	$C_{13}H_{10}INO$
M_r	247.03	323.12
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$
Temperature (K)	296	120
a, b, c (Å)	5.0531 (2), 11.4478 (5), 13.2945 (5)	5.1225 (2), 10.4572 (4), 12.2167 (5)
α, β, γ (°)	90, 93.245 (1), 90	66.034 (2), 78.882 (2), 85.760 (2)
V (Å³)	767.81 (5)	586.76 (4)
Z	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm⁻¹)	4.10	2.71
Crystal size (mm)	0.23 × 0.22 × 0.21	0.23 × 0.22 × 0.21
Data collection		
Diffractometer	Bruker Kappa APEXII DUO	Bruker Kappa APEXII DUO
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.429, 0.456	0.546, 0.570
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5827, 1504, 1461	13292, 2309, 2278
R_{int}	0.021	0.018
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.617	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.014, 0.033, 1.16	0.017, 0.042, 1.08
No. of reflections	1504	2309
No. of parameters	92	145
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å⁻³)	0.45, −0.35	0.81, −0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS14* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012) and *PARST* (Nardelli, 1995).

4. Database survey

A search for the crystal structures of 2-iodobenzamide and 2-iodo-*N*-phenylbenzamide was carried out in the Cambridge Structural Database (Conquest Version 1.17; CSD Version 5.39, last update November 2017; Groom *et al.*, 2016). Compound (I) was found to have been previously reported from film data (IBNZAM; Nakata *et al.*, 1976), but there were no hits for compound (II). Four other related structures were observed: two fluorine-substituted 2-iodobenzamides, FAHSAK and FAHSIS (Nayak *et al.*, 2012) and two nitro substituted 2-iodobenzamides, TAQBIX (Garden *et al.*, 2005) and WAWMAJ (Wardell *et al.*, 2005).

5. Synthesis and crystallization

The synthesis of the title compounds was carried out using a reported procedure (Jursic & Zdravkovski, 1993; Kavala *et al.*, 2012; Mao *et al.*, 2012). Single crystals for both compounds were grown by the slow evaporation method from dichloromethane and hexane (*v/v* 1:1) at low temperature for (I), whereas those for compound (II) were obtained from aceto-
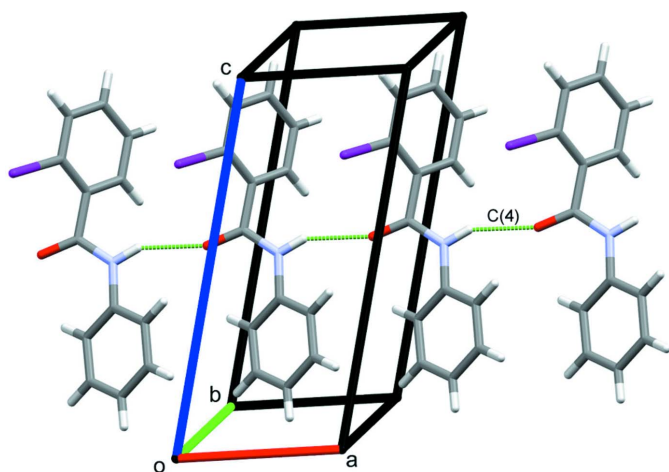
Figure 5
N—H⋯O hydrogen bonds forming chains of molecules of (II) along the *a*-axis direction.
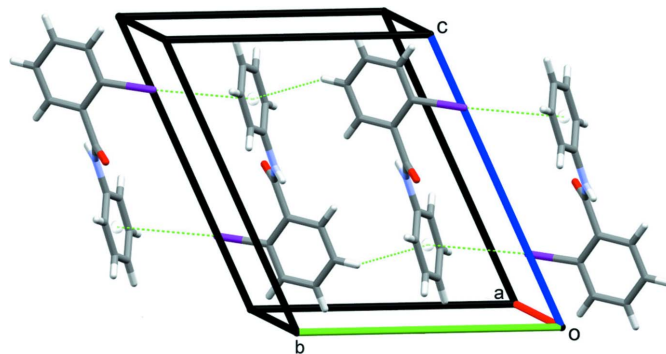
Figure 6
C—I⋯π(ring) and C—H⋯π(ring) contacts generating sheets of molecules of (II) along the *ab* diagonal

nitrile solvent at room temperature. The melting points of (I) and (II) are 398.2 and 419.6 K, respectively. Infra-red (IR) spectra confirm the presence of various functional groups as follows: compound (I) (cm^{-1}): N—H = 3362, 3177, C=O = 1644, C=C = 1581–1470, *ortho*-substituted ring = 734; compound (II) (cm^{-1}): N—H = 3235, Csp^2—H = 3037, C=O = 1646, C=C = 1536–1488, *ortho*-substituted ring = 752, N—H bending = 1597.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were refined using a riding model with d(N—H) = 0.86 Å, U_{iso}(H) = 1.2U_{eq}(N) and d(C—H) = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C) for (I) and d(N—H) = 0.88 Å, U_{iso}(H) = 1.2U_{eq}(N) and d(C—H) = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C) for (II).

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supporting information

Structural analysis of 2-iodobenzamide and 2-iodo-*N*-phenylbenzamide

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Computing details

For both structures, data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS14* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008). Software used to prepare material for publication: *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995) for (I); *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009) for (II).

2-Iodobenzamide (I)

Crystal data

C_7H_6INO	$F(000) = 464$
$M_r = 247.03$	$D_x = 2.137$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 5.0531$ (2) Å	Cell parameters from 1504 reflections
$b = 11.4478$ (5) Å	$\theta = 2.3$–$26.0°$
$c = 13.2945$ (5) Å	$\mu = 4.10$ mm^{-1}
$\beta = 93.245$ (1)°	$T = 296$ K
$V = 767.81$ (5) Å^3	Plate, colorless
$Z = 4$	$0.23 \times 0.22 \times 0.21$ mm

Data collection

Bruker Kappa APEXII DUO diffractometer	5827 measured reflections
Radiation source: fine-focus sealed tube	1504 independent reflections
Graphite monochromator	1461 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.021$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
$T_{min} = 0.429$, $T_{max} = 0.456$	$h = -6 \rightarrow 6$
	$k = -14 \rightarrow 11$
	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.014$	$w = 1/[\sigma^2(F_o^2) + (0.0075P)^2 + 0.6908P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.033$	
$S = 1.16$	$(\Delta/\sigma)_{max} = 0.002$
1504 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
92 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
0 restraints	

Extinction correction: SHELXL2014
(Sheldrick, 2015),
$Fc^*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0170 (5)

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*	$U_{iso}*/U_{eq}$
I1	0.14922 (2)	0.55570 (2)	0.18090 (2)	0.01703 (7)
O1	0.3073 (3)	0.43218 (14)	0.39426 (11)	0.0177 (3)
N1	0.7508 (3)	0.44020 (16)	0.41536 (14)	0.0168 (4)
H1A	0.7438	0.4650	0.4762	0.020*
H1B	0.9018	0.4297	0.3900	0.020*
C5	0.6303 (4)	0.2793 (2)	0.06578 (17)	0.0219 (5)
H5	0.6514	0.2473	0.0024	0.026*
C6	0.7846 (4)	0.23997 (19)	0.14775 (17)	0.0202 (5)
H6	0.9113	0.1824	0.1396	0.024*
C7	0.7504 (4)	0.28652 (19)	0.24225 (17)	0.0165 (4)
H7	0.8555	0.2598	0.2972	0.020*
C2	0.5610 (4)	0.37276 (18)	0.25648 (15)	0.0125 (4)
C1	0.5297 (4)	0.41830 (18)	0.36086 (15)	0.0125 (4)
C4	0.4440 (4)	0.3662 (2)	0.07746 (16)	0.0193 (5)
H4	0.3416	0.3931	0.0219	0.023*
C3	0.4101 (4)	0.41317 (18)	0.17218 (16)	0.0138 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01454 (9)	0.01736 (10)	0.01910 (10)	0.00237 (5)	0.00030 (5)	0.00353 (5)
O1	0.0082 (7)	0.0300 (9)	0.0152 (8)	−0.0007 (6)	0.0019 (5)	−0.0026 (6)
N1	0.0094 (8)	0.0280 (11)	0.0132 (9)	−0.0003 (7)	0.0021 (6)	−0.0044 (8)
C5	0.0286 (12)	0.0200 (11)	0.0177 (12)	−0.0038 (9)	0.0070 (9)	−0.0071 (9)
C6	0.0210 (11)	0.0125 (11)	0.0277 (12)	−0.0010 (9)	0.0085 (9)	−0.0048 (9)
C7	0.0138 (9)	0.0140 (10)	0.0220 (11)	−0.0022 (8)	0.0024 (8)	0.0013 (9)
C2	0.0100 (9)	0.0122 (10)	0.0154 (10)	−0.0034 (7)	0.0019 (7)	−0.0003 (8)
C1	0.0118 (9)	0.0117 (9)	0.0142 (10)	−0.0002 (8)	0.0015 (7)	0.0036 (8)
C4	0.0213 (10)	0.0226 (12)	0.0140 (11)	−0.0042 (9)	−0.0002 (8)	−0.0012 (9)
C3	0.0120 (9)	0.0122 (10)	0.0173 (11)	−0.0019 (8)	0.0025 (8)	0.0005 (8)

Geometric parameters (Å, º)

I1—C3	2.105 (2)	C6—C7	1.385 (3)
O1—C1	1.242 (2)	C6—H6	0.9300

N1—C1	1.321 (3)	C7—C2	1.395 (3)
N1—H1A	0.8600	C7—H7	0.9300
N1—H1B	0.8600	C2—C3	1.398 (3)
C5—C6	1.379 (3)	C2—C1	1.499 (3)
C5—C4	1.384 (3)	C4—C3	1.389 (3)
C5—H5	0.9300	C4—H4	0.9300
C1—N1—H1A	120.0	C7—C2—C3	118.20 (19)
C1—N1—H1B	120.0	C7—C2—C1	118.73 (18)
H1A—N1—H1B	120.0	C3—C2—C1	123.07 (18)
C6—C5—C4	120.2 (2)	O1—C1—N1	122.29 (19)
C6—C5—H5	119.9	O1—C1—C2	121.37 (18)
C4—C5—H5	119.9	N1—C1—C2	116.32 (16)
C5—C6—C7	119.8 (2)	C5—C4—C3	120.0 (2)
C5—C6—H6	120.1	C5—C4—H4	120.0
C7—C6—H6	120.1	C3—C4—H4	120.0
C6—C7—C2	121.1 (2)	C4—C3—C2	120.61 (19)
C6—C7—H7	119.4	C4—C3—I1	117.38 (16)
C2—C7—H7	119.4	C2—C3—I1	121.81 (15)
C4—C5—C6—C7	0.9 (3)	C6—C5—C4—C3	−0.7 (3)
C5—C6—C7—C2	0.2 (3)	C5—C4—C3—C2	−0.6 (3)
C6—C7—C2—C3	−1.5 (3)	C5—C4—C3—I1	174.29 (16)
C6—C7—C2—C1	178.91 (18)	C7—C2—C3—C4	1.7 (3)
C7—C2—C1—O1	−135.1 (2)	C1—C2—C3—C4	−178.75 (18)
C3—C2—C1—O1	45.3 (3)	C7—C2—C3—I1	−172.99 (14)
C7—C2—C1—N1	43.5 (3)	C1—C2—C3—I1	6.6 (3)
C3—C2—C1—N1	−136.1 (2)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C2–C7 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^i	0.86	2.11	2.951 (2)	164
N1—H1*B*···O1^{ii}	0.86	2.05	2.843 (2)	154
C3—I1···*Cg*1^{iii}	2.11 (1)	3.99 (1)	5.877 (2)	148 (1)

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

2-Iodo-*N*-phenylbenzamide (II)

Crystal data

$C_{13}H_{10}INO$	$\gamma = 85.760$ (2)°
$M_r = 323.12$	$V = 586.76$ (4) Å^3
Triclinic, $P\overline{1}$	$Z = 2$
$a = 5.1225$ (2) Å	$F(000) = 312$
$b = 10.4572$ (4) Å	$D_x = 1.829$ Mg m^{-3}
$c = 12.2167$ (5) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\alpha = 66.034$ (2)°	Cell parameters from 2309 reflections
$\beta = 78.882$ (2)°	$\theta = 1.9$–26.0°

$\mu = 2.71$ mm^{-1}

$T = 120$ K

Plate, colorless

$0.23 \times 0.22 \times 0.21$ mm

Data collection

Bruker Kappa APEXII DUO diffractometer	13292 measured reflections
Radiation source: fine-focus sealed tube	2309 independent reflections
Graphite monochromator	2278 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.018$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
	$h = -6 \rightarrow 6$
	$k = -12 \rightarrow 12$
$T_{min} = 0.546$, $T_{max} = 0.570$	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.017$	H-atom parameters constrained
$wR(F^2) = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2 + 0.7193P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
2309 reflections	$(\Delta/\sigma)_{max} < 0.001$
145 parameters	$\Delta\rho_{max} = 0.81$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.48$ 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	−0.30400 (3)	0.03723 (2)	0.77480 (2)	0.01972 (6)
O1	−0.1224 (3)	0.31161 (18)	0.51921 (14)	0.0233 (3)
N1	0.3285 (3)	0.2852 (2)	0.49180 (16)	0.0169 (4)
H1	0.4668	0.2731	0.5279	0.020*
C1	0.0875 (4)	0.2939 (2)	0.55727 (19)	0.0161 (4)
C2	0.0968 (4)	0.2802 (2)	0.68392 (19)	0.0148 (4)
C3	−0.0677 (4)	0.1861 (2)	0.7861 (2)	0.0156 (4)
C4	−0.0629 (4)	0.1793 (2)	0.9014 (2)	0.0194 (4)
H4	−0.1751	0.1151	0.9704	0.023*
C5	0.1069 (4)	0.2670 (2)	0.9157 (2)	0.0206 (4)
H5	0.1091	0.2632	0.9945	0.025*
C6	0.2728 (4)	0.3597 (2)	0.8154 (2)	0.0198 (4)
H6	0.3893	0.4191	0.8255	0.024*
C7	0.2685 (4)	0.3657 (2)	0.7005 (2)	0.0169 (4)
H7	0.3838	0.4289	0.6321	0.020*
C8	0.3800 (4)	0.2938 (2)	0.37055 (19)	0.0159 (4)
C9	0.2215 (4)	0.3717 (2)	0.2855 (2)	0.0180 (4)
H9	0.0683	0.4185	0.3083	0.022*
C10	0.2897 (4)	0.3802 (2)	0.1671 (2)	0.0191 (4)

H10	0.1821	0.4334	0.1089	0.023*
C11	0.5124 (4)	0.3123 (2)	0.1323 (2)	0.0203 (4)
H11	0.5579	0.3190	0.0510	0.024*
C12	0.6677 (4)	0.2343 (2)	0.2180 (2)	0.0209 (5)
H12	0.8204	0.1873	0.1952	0.025*
C13	0.6024 (4)	0.2245 (2)	0.3364 (2)	0.0192 (4)
H13	0.7094	0.1703	0.3945	0.023*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01580 (8)	0.01876 (9)	0.02535 (9)	−0.00291 (5)	−0.00378 (6)	−0.00904 (6)
O1	0.0114 (7)	0.0402 (10)	0.0194 (8)	−0.0006 (7)	−0.0035 (6)	−0.0126 (7)
N1	0.0106 (8)	0.0271 (10)	0.0150 (9)	0.0003 (7)	−0.0026 (7)	−0.0103 (8)
C1	0.0134 (10)	0.0183 (10)	0.0171 (10)	−0.0018 (8)	−0.0013 (8)	−0.0078 (8)
C2	0.0118 (9)	0.0171 (10)	0.0169 (10)	0.0039 (8)	−0.0035 (8)	−0.0084 (8)
C3	0.0109 (9)	0.0172 (10)	0.0214 (11)	0.0004 (8)	−0.0028 (8)	−0.0105 (9)
C4	0.0178 (10)	0.0221 (11)	0.0160 (10)	0.0002 (8)	0.0004 (8)	−0.0069 (9)
C5	0.0207 (11)	0.0270 (12)	0.0174 (10)	0.0026 (9)	−0.0042 (8)	−0.0124 (9)
C6	0.0186 (10)	0.0216 (11)	0.0235 (11)	0.0002 (8)	−0.0063 (9)	−0.0124 (9)
C7	0.0131 (10)	0.0180 (10)	0.0187 (10)	−0.0005 (8)	−0.0013 (8)	−0.0070 (9)
C8	0.0129 (9)	0.0206 (10)	0.0161 (10)	−0.0047 (8)	−0.0003 (8)	−0.0095 (9)
C9	0.0139 (10)	0.0213 (11)	0.0203 (11)	−0.0010 (8)	−0.0018 (8)	−0.0103 (9)
C10	0.0179 (10)	0.0220 (11)	0.0179 (10)	−0.0045 (8)	−0.0046 (8)	−0.0071 (9)
C11	0.0208 (11)	0.0247 (11)	0.0182 (10)	−0.0076 (9)	0.0010 (8)	−0.0121 (9)
C12	0.0152 (10)	0.0256 (12)	0.0259 (12)	−0.0031 (9)	0.0014 (9)	−0.0159 (10)
C13	0.0138 (10)	0.0244 (11)	0.0218 (11)	0.0004 (8)	−0.0046 (8)	−0.0109 (9)

Geometric parameters (Å, º)

I1—C3	2.104 (2)	C6—H6	0.9500
O1—C1	1.225 (3)	C7—H7	0.9500
N1—C1	1.354 (3)	C8—C13	1.392 (3)
N1—C8	1.420 (3)	C8—C9	1.394 (3)
N1—H1	0.8800	C9—C10	1.388 (3)
C1—C2	1.505 (3)	C9—H9	0.9500
C2—C7	1.395 (3)	C10—C11	1.388 (3)
C2—C3	1.399 (3)	C10—H10	0.9500
C3—C4	1.387 (3)	C11—C12	1.388 (3)
C4—C5	1.390 (3)	C11—H11	0.9500
C4—H4	0.9500	C12—C13	1.382 (3)
C5—C6	1.385 (3)	C12—H12	0.9500
C5—H5	0.9500	C13—H13	0.9500
C6—C7	1.384 (3)		
C1—N1—C8	126.37 (18)	C6—C7—C2	120.8 (2)
C1—N1—H1	116.8	C6—C7—H7	119.6
C8—N1—H1	116.8	C2—C7—H7	119.6

O1—C1—N1	124.4 (2)	C13—C8—C9	119.80 (19)
O1—C1—C2	121.64 (19)	C13—C8—N1	117.79 (19)
N1—C1—C2	113.98 (18)	C9—C8—N1	122.38 (19)
C7—C2—C3	118.70 (19)	C10—C9—C8	119.4 (2)
C7—C2—C1	119.60 (19)	C10—C9—H9	120.3
C3—C2—C1	121.68 (18)	C8—C9—H9	120.3
C4—C3—C2	120.61 (19)	C11—C10—C9	121.1 (2)
C4—C3—I1	117.07 (16)	C11—C10—H10	119.5
C2—C3—I1	122.08 (15)	C9—C10—H10	119.5
C3—C4—C5	119.7 (2)	C10—C11—C12	119.0 (2)
C3—C4—H4	120.1	C10—C11—H11	120.5
C5—C4—H4	120.1	C12—C11—H11	120.5
C6—C5—C4	120.3 (2)	C13—C12—C11	120.7 (2)
C6—C5—H5	119.9	C13—C12—H12	119.7
C4—C5—H5	119.9	C11—C12—H12	119.7
C7—C6—C5	119.9 (2)	C12—C13—C8	120.1 (2)
C7—C6—H6	120.1	C12—C13—H13	120.0
C5—C6—H6	120.1	C8—C13—H13	120.0
C8—N1—C1—O1	−0.6 (4)	C5—C6—C7—C2	0.6 (3)
C8—N1—C1—C2	179.69 (19)	C3—C2—C7—C6	−1.2 (3)
O1—C1—C2—C7	−127.2 (2)	C1—C2—C7—C6	177.16 (19)
N1—C1—C2—C7	52.6 (3)	C1—N1—C8—C13	−152.1 (2)
O1—C1—C2—C3	51.1 (3)	C1—N1—C8—C9	29.9 (3)
N1—C1—C2—C3	−129.1 (2)	C13—C8—C9—C10	−0.7 (3)
C7—C2—C3—C4	0.9 (3)	N1—C8—C9—C10	177.34 (19)
C1—C2—C3—C4	−177.47 (19)	C8—C9—C10—C11	0.1 (3)
C7—C2—C3—I1	−173.28 (15)	C9—C10—C11—C12	0.3 (3)
C1—C2—C3—I1	8.4 (3)	C10—C11—C12—C13	−0.1 (3)
C2—C3—C4—C5	0.1 (3)	C11—C12—C13—C8	−0.4 (3)
I1—C3—C4—C5	174.51 (16)	C9—C8—C13—C12	0.8 (3)
C3—C4—C5—C6	−0.7 (3)	N1—C8—C13—C12	−177.3 (2)
C4—C5—C6—C7	0.4 (3)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C8–C13 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1ⁱ	0.88	2.15	2.942 (2)	150
C3—I1···Cg2ⁱⁱ	2.10 (1)	3.83 (1)	5.816 (2)	156 (1)
C6—H6···Cg2ⁱⁱⁱ	0.95	2.81	3.627 (2)	144

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1.