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4-Iodo-*N*-(phenylsulfonyl)benzamide hemihydrate

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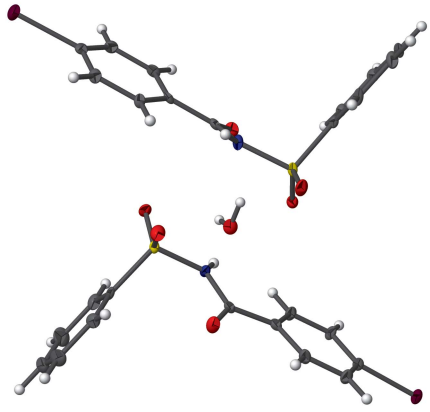
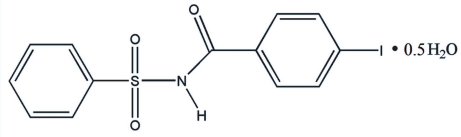
Structural data: full structural data are available from iucrdata.iucr.org

In the title hemihydrate, $2C_{13}H_{10}INO_3S\cdot H_2O$, there are two organic molecules (*A* and *B*) and one water molecule in the asymmetric unit. The benzene rings are inclined to one another by 77.98 (1)° in *A* and 79.81 (9)° in *B*. The *A* and *B* molecules are connected through a water molecule *via* N—H···O and O—H···O hydrogen bonds. In the extended structure, the *A* molecules are interlinked *via* two water molecules through O—H···O hydrogen bonds to generate $R_4^4(12)$ loops. Further, the *A* and *B* molecules are linked by N—H···O hydrogen bonds, and thus an [010] chain is formed. Several C—H···O interactions extend the chains into sheet lying parallel to the *ab*-plane. The sheets are further extended into a three dimensional architecture *via* a C—H···π interaction.

3D view



Chemical scheme



Structure description

In continuation of our work on the synthesis and crystal structures of *N*-(phenylsulfonyl)arylamides (Suchetan *et al.*, 2009, 2010; Gowda *et al.*, 2009), the title compound was synthesized and we report herein on its crystal structure.

The title hemihydrate (Fig. 1) contains two molecules (*A* and *B*) in the asymmetric unit. The benzene rings are inclined to one another by 77.98 (1)° in *A* and 79.81 (9)° in *B*. The *A* and *B* molecules are interconnected through a water molecule *via* N1—H*N*1···O7, O7—H1*O*7···O6 and O7—H1*O*7···O5 hydrogen bonds (Table 1). The bifurcated O7—H1*O*7···(O5,O6) hydrogen bonds form $R_1^2(6)$ rings (Fig. 1). The *A* molecules in the neighboring asymmetric units are interlinked *via* two water molecules through O7—H2*O*7···O1^{ii} (Table 1) hydrogen bonds to form an $R_4^4(12)$ loop. Further, the *A* and *B* molecules in adjacent $R_4^4(12)$ ring motifs are linked by N2—H*N*2···O2^{i} (Table 1)

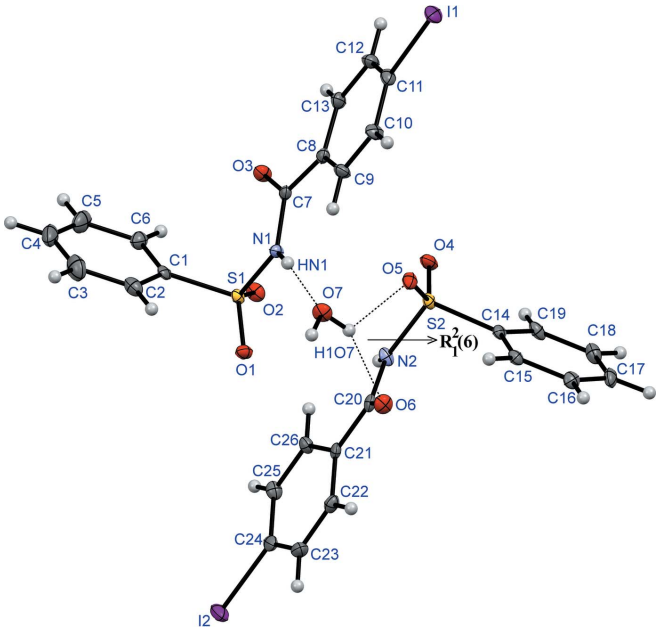


Figure 1
A view of the molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. The N—H···O and O—H···O hydrogen bonds (dashed lines, see Table 1) are also shown.

hydrogen bonds, and thus, a chain is observed parallel to the *b*-axis direction (Fig. 2). Further, C9—H9···O7, C18—H18···O4^{iii} and C26—H26···O2^{i} (Table 1) interactions extend the chains into a sheets in the *ab* plane (Fig. 3). The sheets are further extended into a three-dimensional architecture *via* C17—H17···π^{iv} interactions involving the π electrons of the iodobenzene ring of molecule *B* (Table 1).

Synthesis and crystallization

The title compound was prepared by refluxing a mixture of 4-iodobenzoic acid (3 mmol), benzenesulfonamide (3 mmol) and phosphorus oxychloride (7 ml) for 3 h on a water bath. The resultant mixture was cooled and poured into ice-cold water. The solid obtained was filtered, washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. It was later filtered, dried and recrystallized (m.p. = 460 K). Colourless prisms were obtained by slow evaporation of a solution of the compound in methanol (with a few drops of added water).

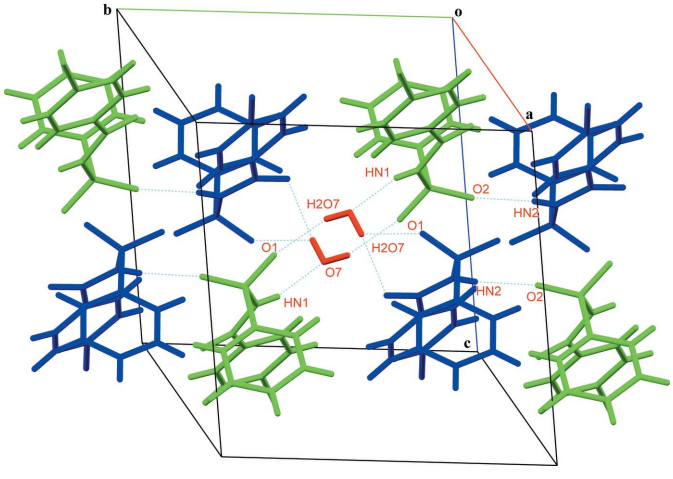


Figure 2
Generation of chains along [010] *via* several N—H···O and O—H···O hydrogen bonds (dashed lines, see Table 1).

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

Cg is the centroid of the iodobenzene ring (C21–C26) of molecule *B*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···O2^{i}	0.84	2.12	2.9271	160
N1—H*N*1···O7	0.81	2.01	2.7894	163
O7—H2*O*7···O1^{ii}	0.82	2.09	2.8507	154
O7—H1*O*7···O5	0.83	2.32	2.8283	121
O7—H1*O*7···O6	0.83	2.23	2.9898	152
C9—H9···O7	0.95	2.37	3.2680	158
C18—H18···O4^{iii}	0.95	2.58	3.429 (5)	149
C26—H26···O2^{i}	0.95	2.59	3.376 (5)	140
C17—H17···*Cg*^{iv}	0.95	2.88	3.7194	148

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y, -z+1$; (iv) $x-1, y, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_{13}H_{10}INO_3S\cdot H_2O$
M_r	792.37
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, *b*, *c* (Å)	10.6311 (5), 11.0403 (5), 12.0340 (6)
α, β, γ (°)	97.594 (2), 92.173 (2), 99.423 (1)
V (Å^3)	1378.59 (11)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	19.75
Crystal size (mm)	0.22 × 0.11 × 0.08
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.111, 0.206
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14470, 4556, 4351
R_{int}	0.052
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.114, 1.07
No. of reflections	4556
No. of parameters	368
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.23, −1.18

Computer programs: *APEX2* and *SAINT-Plus* (Bruker, 2009), *SHELXT2016/4* (Sheldrick, 2015*a*), *SHELXL2016/4* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2008).

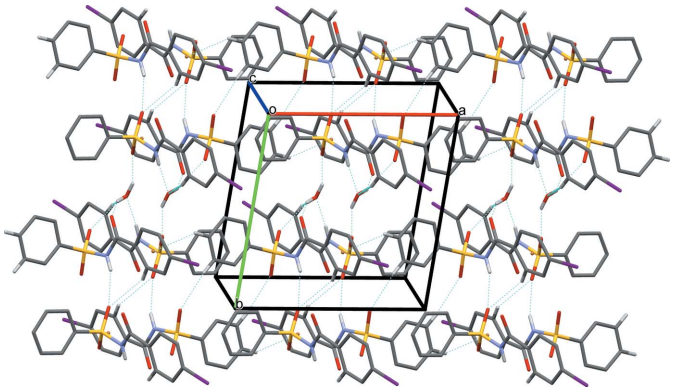


Figure 3
A view along the *c* axis of the crystal packing of the title compound, showing the N—H···O, O—H···O and C—H···O hydrogen bonds (dashed lines; see Table 1). For clarity, only H atoms involved in hydrogen bonding have been included.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170149 [https://doi.org/10.1107/S2414314617001493]

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Crystal data

$2C_{13}H_{10}INO_3S·H_2O$
M_r = 792.37
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 10.6311 (5) Å
b = 11.0403 (5) Å
c = 12.0340 (6) Å
α = 97.594 (2)°
β = 92.173 (2)°
γ = 99.423 (1)°
V = 1378.59 (11) Å^3
Z = 2
$F(000)$ = 772
Prism
D_x = 1.909 Mg m^{-3}
Melting point: 460 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 175 reflections
θ = 3.7–64.5°
μ = 19.75 mm^{-1}
T = 173 K
Prism, colourless
0.22 × 0.11 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Radiation source: CuKα
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.111, T_{max} = 0.206
14470 measured reflections
4556 independent reflections
4351 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 64.5°, θ_{min} = 3.7°
h = −12→12
k = −12→12
l = −13→12
1 standard reflections every 2 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.07
4556 reflections
368 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0797P)^2 + 0.2627P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.90191 (2)	0.36213 (2)	−0.13476 (2)	0.02152 (13)
I2	0.23891 (2)	0.22303 (3)	0.99991 (2)	0.02462 (14)
S1	0.36863 (8)	0.18597 (8)	0.38822 (7)	0.0102 (2)
S2	0.77577 (8)	0.20298 (8)	0.46211 (7)	0.0113 (2)
O5	0.7584 (3)	0.2982 (3)	0.3964 (2)	0.0148 (6)
O7	0.5953 (3)	0.4761 (2)	0.3928 (2)	0.0171 (6)
O3	0.4363 (2)	0.0618 (2)	0.1777 (2)	0.0156 (6)
O2	0.3857 (3)	0.0650 (2)	0.4095 (2)	0.0163 (6)
O1	0.3821 (3)	0.2831 (2)	0.4811 (2)	0.0140 (6)
O6	0.6832 (3)	0.4039 (2)	0.6098 (2)	0.0168 (6)
O4	0.7648 (3)	0.0778 (3)	0.4096 (2)	0.0170 (6)
N1	0.4739 (3)	0.2383 (3)	0.3017 (3)	0.0112 (7)
N2	0.6669 (3)	0.1963 (3)	0.5582 (3)	0.0122 (6)
C15	0.9731 (4)	0.3725 (4)	0.5712 (3)	0.0126 (7)
H15	0.926916	0.434422	0.552424	0.015*
C1	0.2180 (3)	0.1746 (3)	0.3169 (3)	0.0125 (7)
C14	0.9236 (4)	0.2471 (3)	0.5399 (3)	0.0116 (7)
C24	0.3720 (4)	0.2426 (4)	0.8768 (3)	0.0164 (8)
C12	0.7210 (4)	0.1779 (4)	−0.0283 (3)	0.0173 (8)
H12	0.743547	0.121332	−0.087657	0.021*
C10	0.7450 (4)	0.3854 (4)	0.0721 (3)	0.0154 (8)
H10	0.784176	0.470125	0.081032	0.019*
C20	0.6363 (3)	0.2989 (3)	0.6239 (3)	0.0120 (7)
C21	0.5443 (3)	0.2734 (3)	0.7113 (3)	0.0115 (7)
C8	0.5987 (4)	0.2195 (4)	0.1336 (3)	0.0124 (8)
C16	1.0901 (4)	0.4050 (4)	0.6297 (3)	0.0151 (8)
H16	1.125122	0.490056	0.651777	0.018*
C7	0.4972 (3)	0.1648 (3)	0.2042 (3)	0.0115 (7)
C19	0.9877 (4)	0.1553 (4)	0.5686 (3)	0.0154 (8)
H19	0.951207	0.070383	0.548274	0.018*
C23	0.4521 (4)	0.3553 (4)	0.8779 (3)	0.0176 (8)
H23	0.448327	0.421848	0.935780	0.021*
C25	0.3778 (4)	0.1433 (4)	0.7931 (3)	0.0148 (8)
H25	0.323712	0.065693	0.792743	0.018*
C11	0.7758 (4)	0.3025 (4)	−0.0153 (3)	0.0155 (8)
C6	0.1536 (4)	0.0613 (4)	0.2665 (3)	0.0186 (8)
H6	0.189454	−0.011585	0.270213	0.022*
C9	0.6569 (4)	0.3438 (4)	0.1463 (3)	0.0152 (8)
H9	0.635821	0.400468	0.206341	0.018*

C22	0.5372 (4)	0.3713 (4)	0.7955 (3)	0.0150 (8)
H22	0.591048	0.449034	0.796067	0.018*
C17	1.1573 (4)	0.3134 (4)	0.6568 (3)	0.0176 (8)
H17	1.239003	0.336432	0.695619	0.021*
C2	0.1678 (4)	0.2839 (4)	0.3122 (3)	0.0194 (8)
H2	0.213500	0.361512	0.347460	0.023*
C26	0.4635 (4)	0.1603 (4)	0.7114 (3)	0.0137 (8)
H26	0.467745	0.093534	0.653865	0.016*
C18	1.1058 (4)	0.1885 (4)	0.6273 (4)	0.0192 (9)
H18	1.151187	0.126474	0.647265	0.023*
C13	0.6336 (4)	0.1376 (4)	0.0459 (3)	0.0162 (8)
H13	0.596126	0.052405	0.037462	0.019*
C4	−0.0152 (4)	0.1618 (5)	0.2050 (4)	0.0301 (11)
H4	−0.095970	0.157034	0.166620	0.036*
C3	0.0513 (5)	0.2767 (5)	0.2559 (4)	0.0297 (11)
H3	0.016110	0.349761	0.251479	0.036*
C5	0.0360 (4)	0.0544 (5)	0.2103 (4)	0.0287 (10)
H5	−0.009541	−0.023486	0.175348	0.034*
H2O7	0.578 (6)	0.543 (3)	0.420 (5)	0.040 (16)*
H1O7	0.643 (4)	0.457 (5)	0.441 (4)	0.026 (14)*
HN2	0.637 (4)	0.127 (3)	0.577 (4)	0.017 (11)*
HN1	0.507 (5)	0.310 (3)	0.315 (5)	0.030 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01479 (19)	0.0317 (2)	0.0166 (2)	−0.00216 (12)	0.00650 (12)	0.00403 (13)
I2	0.0180 (2)	0.0412 (2)	0.0176 (2)	0.00979 (14)	0.00791 (13)	0.00722 (14)
S1	0.0087 (4)	0.0085 (4)	0.0127 (5)	−0.0003 (3)	0.0025 (3)	0.0011 (3)
S2	0.0082 (4)	0.0102 (4)	0.0149 (5)	−0.0008 (3)	0.0027 (3)	0.0013 (3)
O5	0.0111 (13)	0.0200 (14)	0.0142 (14)	0.0009 (10)	0.0017 (10)	0.0072 (11)
O7	0.0195 (15)	0.0094 (14)	0.0214 (15)	0.0017 (11)	0.0022 (12)	−0.0003 (11)
O3	0.0157 (13)	0.0102 (13)	0.0189 (14)	−0.0015 (10)	0.0041 (11)	−0.0020 (10)
O2	0.0188 (14)	0.0127 (13)	0.0193 (14)	0.0051 (10)	0.0038 (11)	0.0053 (11)
O1	0.0148 (14)	0.0138 (13)	0.0116 (14)	−0.0010 (10)	0.0021 (11)	−0.0011 (10)
O6	0.0174 (14)	0.0099 (14)	0.0212 (15)	−0.0022 (10)	0.0016 (11)	0.0013 (11)
O4	0.0148 (14)	0.0160 (14)	0.0175 (14)	−0.0010 (10)	0.0057 (11)	−0.0047 (11)
N1	0.0099 (16)	0.0115 (17)	0.0101 (16)	−0.0021 (12)	0.0021 (12)	−0.0012 (13)
N2	0.0104 (15)	0.0081 (16)	0.0185 (17)	0.0000 (12)	0.0048 (12)	0.0043 (13)
C15	0.0119 (18)	0.0126 (19)	0.0138 (19)	0.0015 (14)	0.0044 (14)	0.0035 (15)
C1	0.0090 (18)	0.0163 (19)	0.0113 (18)	−0.0009 (14)	0.0050 (14)	0.0012 (14)
C14	0.0087 (18)	0.0136 (18)	0.0112 (18)	−0.0016 (14)	0.0029 (14)	0.0014 (15)
C24	0.014 (2)	0.027 (2)	0.012 (2)	0.0100 (16)	−0.0006 (15)	0.0041 (16)
C12	0.016 (2)	0.020 (2)	0.0141 (19)	0.0016 (16)	0.0046 (15)	−0.0032 (16)
C10	0.015 (2)	0.016 (2)	0.014 (2)	−0.0032 (15)	0.0059 (15)	0.0028 (15)
C20	0.0074 (17)	0.0136 (19)	0.0149 (19)	0.0012 (14)	−0.0026 (14)	0.0033 (14)
C21	0.0065 (17)	0.0140 (18)	0.0140 (19)	0.0022 (14)	−0.0023 (14)	0.0019 (14)
C8	0.0099 (18)	0.0134 (18)	0.0136 (19)	0.0026 (14)	−0.0015 (14)	0.0004 (15)

C16	0.0136 (19)	0.0151 (19)	0.016 (2)	−0.0016 (15)	0.0029 (15)	0.0044 (15)
C7	0.0085 (17)	0.0123 (19)	0.0131 (19)	0.0029 (14)	−0.0016 (14)	−0.0010 (15)
C19	0.0120 (19)	0.0122 (18)	0.022 (2)	0.0012 (14)	0.0077 (15)	0.0030 (15)
C23	0.016 (2)	0.021 (2)	0.014 (2)	0.0039 (15)	−0.0012 (15)	−0.0030 (15)
C25	0.0134 (19)	0.0140 (19)	0.018 (2)	0.0022 (15)	0.0025 (15)	0.0066 (15)
C11	0.0116 (18)	0.022 (2)	0.0141 (19)	0.0011 (15)	0.0025 (15)	0.0065 (16)
C6	0.015 (2)	0.021 (2)	0.017 (2)	−0.0025 (15)	0.0013 (15)	0.0016 (16)
C9	0.0150 (19)	0.016 (2)	0.0139 (19)	0.0038 (15)	0.0050 (15)	−0.0016 (15)
C22	0.0132 (19)	0.0127 (19)	0.017 (2)	0.0001 (14)	−0.0033 (15)	−0.0005 (15)
C17	0.0081 (18)	0.027 (2)	0.019 (2)	0.0012 (15)	0.0022 (15)	0.0079 (16)
C2	0.019 (2)	0.021 (2)	0.020 (2)	0.0065 (16)	0.0074 (16)	0.0053 (17)
C26	0.0114 (18)	0.0141 (19)	0.016 (2)	0.0041 (14)	0.0030 (15)	0.0016 (15)
C18	0.013 (2)	0.022 (2)	0.024 (2)	0.0056 (16)	0.0046 (16)	0.0071 (17)
C13	0.0110 (18)	0.018 (2)	0.017 (2)	−0.0016 (14)	0.0012 (15)	−0.0022 (15)
C4	0.013 (2)	0.053 (3)	0.023 (2)	0.001 (2)	0.0009 (17)	0.009 (2)
C3	0.023 (2)	0.037 (3)	0.035 (3)	0.014 (2)	0.003 (2)	0.013 (2)
C5	0.017 (2)	0.040 (3)	0.024 (2)	−0.0112 (19)	−0.0010 (18)	0.0030 (19)

Geometric parameters (Å, º)

I1—C11	2.099 (4)	C10—H10	0.9500
I2—C24	2.094 (4)	C20—C21	1.485 (6)
S1—O1	1.428 (3)	C21—C22	1.395 (6)
S1—O2	1.432 (3)	C21—C26	1.396 (6)
S1—N1	1.645 (3)	C8—C9	1.396 (6)
S1—C1	1.766 (4)	C8—C13	1.399 (6)
S2—O4	1.426 (3)	C8—C7	1.497 (6)
S2—O5	1.427 (3)	C16—C17	1.396 (6)
S2—N2	1.666 (3)	C16—H16	0.9500
S2—C14	1.761 (4)	C19—C18	1.388 (6)
O7—H2O7	0.82 (2)	C19—H19	0.9500
O7—H1O7	0.83 (2)	C23—C22	1.376 (6)
O3—C7	1.210 (5)	C23—H23	0.9500
O6—C20	1.220 (5)	C25—C26	1.376 (6)
N1—C7	1.390 (5)	C25—H25	0.9500
N1—HN1	0.81 (3)	C6—C5	1.385 (6)
N2—C20	1.386 (5)	C6—H6	0.9500
N2—HN2	0.84 (3)	C9—H9	0.9500
C15—C16	1.375 (6)	C22—H22	0.9500
C15—C14	1.394 (5)	C17—C18	1.391 (6)
C15—H15	0.9500	C17—H17	0.9500
C1—C6	1.375 (6)	C2—C3	1.375 (7)
C1—C2	1.404 (6)	C2—H2	0.9500
C14—C19	1.383 (5)	C26—H26	0.9500
C24—C23	1.387 (6)	C18—H18	0.9500
C24—C25	1.398 (6)	C13—H13	0.9500
C12—C13	1.376 (6)	C4—C5	1.392 (7)
C12—C11	1.389 (6)	C4—C3	1.397 (7)

C12—H12	0.9500	C4—H4	0.9500
C10—C9	1.384 (6)	C3—H3	0.9500
C10—C11	1.385 (6)	C5—H5	0.9500

O1—S1—O2	118.27 (17)	O3—C7—N1	120.8 (3)
O1—S1—N1	104.13 (17)	O3—C7—C8	122.0 (3)
O2—S1—N1	110.25 (17)	N1—C7—C8	117.2 (3)
O1—S1—C1	109.10 (17)	C14—C19—C18	119.3 (4)
O2—S1—C1	108.84 (17)	C14—C19—H19	120.3
N1—S1—C1	105.46 (17)	C18—C19—H19	120.3
O4—S2—O5	120.03 (17)	C22—C23—C24	120.3 (4)
O4—S2—N2	103.98 (16)	C22—C23—H23	119.9
O5—S2—N2	109.06 (16)	C24—C23—H23	119.9
O4—S2—C14	109.29 (17)	C26—C25—C24	118.7 (4)
O5—S2—C14	108.55 (17)	C26—C25—H25	120.7
N2—S2—C14	104.88 (17)	C24—C25—H25	120.7
H2O7—O7—H1O7	105 (6)	C10—C11—C12	120.9 (4)
C7—N1—S1	121.4 (3)	C10—C11—I1	121.1 (3)
C7—N1—HN1	121 (4)	C12—C11—I1	118.0 (3)
S1—N1—HN1	117 (4)	C1—C6—C5	119.3 (4)
C20—N2—S2	124.3 (3)	C1—C6—H6	120.3
C20—N2—HN2	116 (3)	C5—C6—H6	120.3
S2—N2—HN2	119 (3)	C10—C9—C8	120.6 (4)
C16—C15—C14	118.9 (4)	C10—C9—H9	119.7
C16—C15—H15	120.6	C8—C9—H9	119.7
C14—C15—H15	120.6	C23—C22—C21	120.1 (4)
C6—C1—C2	121.6 (4)	C23—C22—H22	120.0
C6—C1—S1	120.2 (3)	C21—C22—H22	120.0
C2—C1—S1	118.3 (3)	C18—C17—C16	120.6 (4)
C19—C14—C15	121.6 (4)	C18—C17—H17	119.7
C19—C14—S2	118.6 (3)	C16—C17—H17	119.7
C15—C14—S2	119.8 (3)	C3—C2—C1	118.9 (4)
C23—C24—C25	120.5 (4)	C3—C2—H2	120.5
C23—C24—I2	119.4 (3)	C1—C2—H2	120.5
C25—C24—I2	120.0 (3)	C25—C26—C21	121.4 (4)
C13—C12—C11	119.1 (4)	C25—C26—H26	119.3
C13—C12—H12	120.4	C21—C26—H26	119.3
C11—C12—H12	120.4	C19—C18—C17	119.5 (4)
C9—C10—C11	119.5 (4)	C19—C18—H18	120.3
C9—C10—H10	120.2	C17—C18—H18	120.3
C11—C10—H10	120.2	C12—C13—C8	121.3 (4)
O6—C20—N2	121.1 (3)	C12—C13—H13	119.3
O6—C20—C21	122.6 (3)	C8—C13—H13	119.3
N2—C20—C21	116.3 (3)	C5—C4—C3	120.5 (4)
C22—C21—C26	119.1 (4)	C5—C4—H4	119.8
C22—C21—C20	116.8 (3)	C3—C4—H4	119.8
C26—C21—C20	124.1 (3)	C2—C3—C4	119.9 (4)
C9—C8—C13	118.5 (4)	C2—C3—H3	120.0

C9—C8—C7	125.7 (3)	C4—C3—H3	120.0
C13—C8—C7	115.8 (3)	C6—C5—C4	119.8 (4)
C15—C16—C17	120.1 (4)	C6—C5—H5	120.1
C15—C16—H16	119.9	C4—C5—H5	120.1
C17—C16—H16	119.9		

O1—S1—N1—C7	174.5 (3)	C15—C14—C19—C18	−1.7 (6)
O2—S1—N1—C7	46.7 (3)	S2—C14—C19—C18	178.3 (3)
C1—S1—N1—C7	−70.6 (3)	C25—C24—C23—C22	1.0 (6)
O4—S2—N2—C20	−174.6 (3)	I2—C24—C23—C22	−177.8 (3)
O5—S2—N2—C20	−45.4 (3)	C23—C24—C25—C26	−0.7 (6)
C14—S2—N2—C20	70.7 (3)	I2—C24—C25—C26	178.0 (3)
O1—S1—C1—C6	−146.8 (3)	C9—C10—C11—C12	−1.1 (6)
O2—S1—C1—C6	−16.4 (4)	C9—C10—C11—I1	176.9 (3)
N1—S1—C1—C6	101.9 (3)	C13—C12—C11—C10	1.0 (6)
O1—S1—C1—C2	34.0 (4)	C13—C12—C11—I1	−177.1 (3)
O2—S1—C1—C2	164.4 (3)	C2—C1—C6—C5	−0.4 (6)
N1—S1—C1—C2	−77.3 (3)	S1—C1—C6—C5	−179.5 (3)
C16—C15—C14—C19	1.5 (6)	C11—C10—C9—C8	−0.2 (6)
C16—C15—C14—S2	−178.5 (3)	C13—C8—C9—C10	1.4 (6)
O4—S2—C14—C19	−18.8 (3)	C7—C8—C9—C10	−176.6 (4)
O5—S2—C14—C19	−151.4 (3)	C24—C23—C22—C21	−0.9 (6)
N2—S2—C14—C19	92.1 (3)	C26—C21—C22—C23	0.6 (5)
O4—S2—C14—C15	161.2 (3)	C20—C21—C22—C23	178.6 (3)
O5—S2—C14—C15	28.6 (4)	C15—C16—C17—C18	−1.5 (6)
N2—S2—C14—C15	−87.8 (3)	C6—C1—C2—C3	0.1 (6)
S2—N2—C20—O6	4.8 (5)	S1—C1—C2—C3	179.2 (3)
S2—N2—C20—C21	−175.2 (2)	C24—C25—C26—C21	0.5 (6)
O6—C20—C21—C22	−15.9 (5)	C22—C21—C26—C25	−0.4 (5)
N2—C20—C21—C22	164.2 (3)	C20—C21—C26—C25	−178.3 (3)
O6—C20—C21—C26	162.1 (3)	C14—C19—C18—C17	0.3 (6)
N2—C20—C21—C26	−17.9 (5)	C16—C17—C18—C19	1.3 (6)
C14—C15—C16—C17	0.1 (6)	C11—C12—C13—C8	0.3 (6)
S1—N1—C7—O3	3.4 (5)	C9—C8—C13—C12	−1.5 (6)
S1—N1—C7—C8	−177.6 (3)	C7—C8—C13—C12	176.7 (3)
C9—C8—C7—O3	167.6 (4)	C1—C2—C3—C4	0.4 (7)
C13—C8—C7—O3	−10.4 (5)	C5—C4—C3—C2	−0.5 (7)
C9—C8—C7—N1	−11.4 (5)	C1—C6—C5—C4	0.3 (6)
C13—C8—C7—N1	170.6 (3)	C3—C4—C5—C6	0.2 (7)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the iodobenzene ring (C21–C26) of molecule *B*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···O2^{i}	0.84	2.12	2.9271	160
N1—H*N*1···O7	0.81	2.01	2.7894	163
O7—H2*O*7···O1^{ii}	0.82	2.09	2.8507	154
O7—H1*O*7···O5	0.83	2.32	2.8283	121

O7—H1*O*7···O6	0.83	2.23	2.9898	152
C9—H9···O7	0.95	2.37	3.2680	158
C18—H18···O4^{iii}	0.95	2.58	3.429 (5)	149
C26—H26···O2^{i}	0.95	2.59	3.376 (5)	140
C17—H17···*Cg*^{iv}	0.95	2.88	3.7194	148

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