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ISSN 2414-3146

# 4-Iodo-*N*-(*o*-tolylsulfonyl)benzamide

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Received 20 December 2016
Accepted 21 December 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

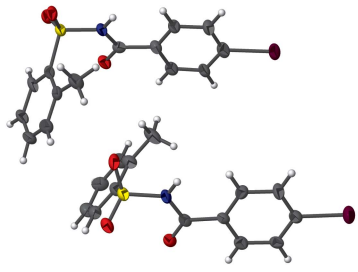
**Keywords:** crystal structure; sulfonamides; benzamide; *o*-tolylsulfony; hydrogen bonding; C—H···$\pi$ interactions.

**CCDC reference**: 1523975

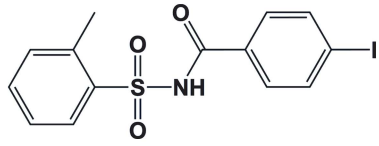
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_{14}H_{12}INO_3S$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The dihedral angle between the two aryl rings is 83.1 (4)° in molecule *A* and 79.8 (4)° in molecule *B*. In the crystal, the two molecules are linked by a pair of N—H···O hydrogen bonds, forming an *A*–*B* dimer with an $R_2^2(8)$ ring motif. The dimer is further strengthened by a pair of C—H···O hydrogen bonds with an $R_2^2(14)$ motif. Another pair of C—H···O interactions assembles these dimers along the diagonal of the *bc* plane, forming ribbons. Adjacent ribbons are connected by C—H···$\pi_{aryl}$ interactions between the *A* molecules, and thus the overall supramolecular architecture is one-dimensional.

**3D view**



**Chemical scheme**




## Structure description

Sulfonamide and amide moieties play a significant role as key constituents in a number of biologically active molecules (Mohan *et al.*, 2013; Manojkumar *et al.*, 2013; Hamad & Abed, 2014). In recent years, *N*-(arylsulfonyl)-arylamides have received much attention as they constitute an important class of drugs for Alzheimer's disease (Hasegawa & Yamamoto, 2000), anti-bacterial inhibitors of tRNA synthetases (Banwell *et al.*, 2000), antagonists for angiotensin II (Chang *et al.*, 1994) and as leukotriene D4-receptors (Musser *et al.*, 1990). Further, *N*-(arylsulfonyl)-arylamides are known as potent anti-tumour agents against a broad spectrum of human tumour xenografts (colon, lung, breast, ovary and prostate) in nude mice (Mader *et al.*, 2005). In view of the importance of *N*-(arylsulfonyl)-arylamides and in continuation of our work on the synthesis and crystal structures of *N*-(2-methylphenylsulfonyl)-arylamides (Suchetan *et al.*, 2010*a*,*b*; Gowda *et al.*, 2010; Suchetan *et al.*, 2011), the title compound was synthesized and we report herein on its crystal structure.

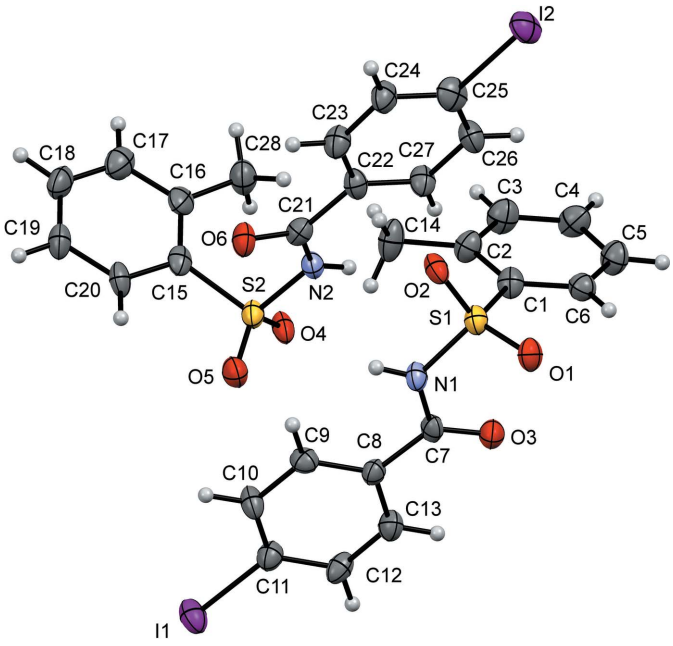



**Figure 1**
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

The asymmetric unit of the title compound, Fig. 1, contains two molecules [*A* (N1) and *B* N2)], similar to the situation observed for *N*-(4-chlorobenzoyl)-2-methylbenzenesulfonamide (Suchetan *et al.*, 2010*b*) and *N*-(4-methylbenzoyl)-2-methylbenzenesulfonamide (Gowda *et al.*, 2010). However, in the crystal structures of *N*-(benzoyl)-2-methylbenzenesulfonamide (Suchetan *et al.*, 2010*a*) and *N*-(4-nitrobenzoyl)-2-methylbenzenesulfonamide (Suchetan *et al.*, 2011), there is only one molecule in the asymmetric unit. The dihedral angles between the two aryl rings are 83.1 (4) and 79.8 (4)° in molecules *A* and *B*, respectively, while the corresponding angle is 73.9 (1)°in *N*-(benzoyl)-2-methylbenzenesulfonamide, 89.4 (1) and 82.4 (1)° in the two molecules of *N*-(4-chlorobenzoyl)-2-methylbenzenesulfonamide, 88.1 (1) and 83.5 (1)° in the two molecules of *N*-(4-methylbenzoyl)-2-methylbenzenesulfonamide, and 83.8 (2)°in *N*-(4-nitrobenzoyl)-2-methylbenzenesulfonamide. In both molecules of the title compound, the *ortho*-methyl substituent is *syn* to N—H bond in the central –C—$SO_2$—N(H)—C(O)– segment, similar to that observed in all the reported structures, the only exception being *N*-(4-methylbenzoyl)-2-methylbenzenesulfonamide, where the conformation is *anti*.

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

*Cg* is the centroid of the iodobenzene ring (C8–C13) of molecule *A*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.88 | 2.06 | 2.900 (10) | 158 |
| N2—H2···O2$^{i}$ | 0.88 | 2.12 | 2.970 (10) | 161 |
| C9—H9···O4$^{i}$ | 0.95 | 2.36 | 3.301 (10) | 170 |
| C13—H13···O6$^{ii}$ | 0.95 | 2.56 | 3.378 (11) | 144 |
| C23—H23···O3$^{ii}$ | 0.95 | 2.40 | 3.201 (11) | 142 |
| C27—H27···O2$^{i}$ | 0.95 | 2.51 | 3.428 (9) | 163 |
| C4—H4···*Cg*$^{iii}$ | 0.93 | 2.81 | 3.656 (11) | 151 |

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

The crystal structure, features two N—H···O hydrogen bonds, namely, N1—H1···O4$^{i}$ and N2—H2···O2$^{i}$ (Table 1), linking the *A* and *B* molecules and resulting in an $R_2^2(8)$ dimer. This arrangement is further strengthened by C9—H9···O4$^{i}$ and C27—H27···O2$^{i}$ hydrogen bonds (Table 1), with an $R_2^2(14)$ ring motif (Fig. 2). Further, another pair of C—H···O interactions, C13—H13···O6$^{ii}$ and C23—H23···O3$^{ii}$, assemble these dimers along the diagonal of the *bc* plane forming ribbons (Fig. 3, Table 1). Adjacent ribbons are connected by C4—H4···$\pi_{aryl}$ (the $\pi$-electron system of the iodobenzene ring of molecule *A*) interactions between the *A* molecules (Fig. 4, Table 1). Thus, the overall supramolecular architecture is one-dimensional. In the structures mentioned above, the assembly of molecules is only due to the N—H···O

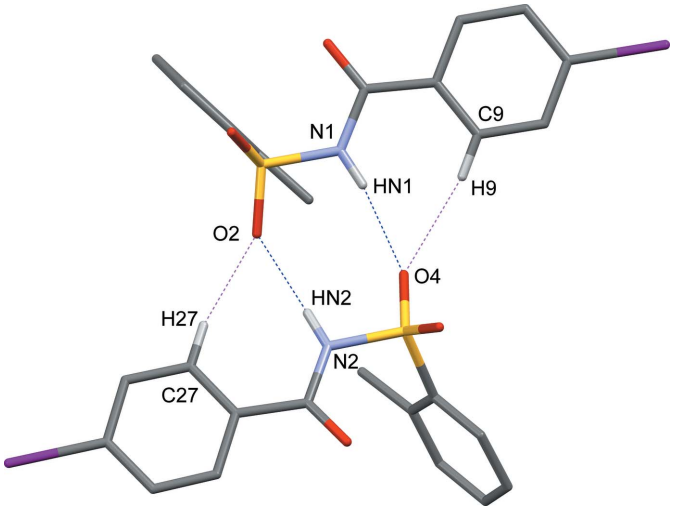



**Figure 2**
A view of the $R_2^2(8)$ and $R_2^2(14)$ dimeric patterns displayed in the crystal structure of the title compound, resulting from N—H···O hydrogen bonds and C—H···O interactions, respectively (dashed lines, see Table 1).

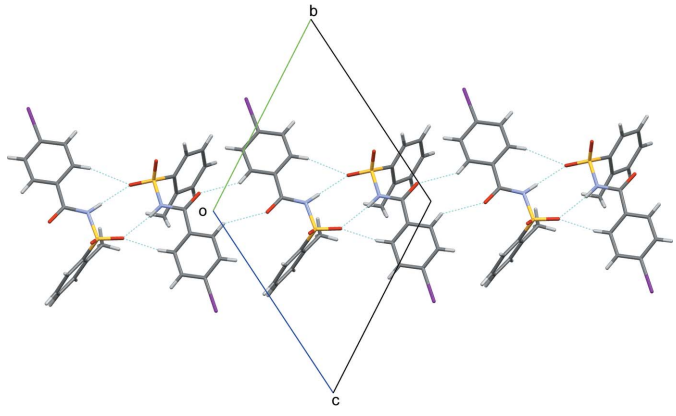



**Figure 3**
Generation of the ribbons *via* C—H···O intermolecular interactions (dashed lines, see Table 1).

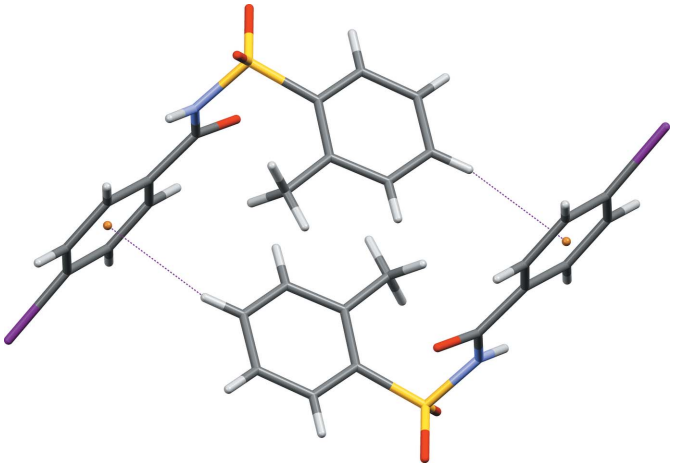


**Figure 4**
A view of the C—H···$\pi_{aryl}$ interactions observed in the crystal structure of the title compound (dashed lines, see Table 1).

hydrogen-bonded $R_2^2(8)$ rings or $C(4)$ chains that result in either zero- or one-dimensional architectures.

## Synthesis and crystallization

The title compound was prepared by refluxing a mixture of 4-iodobenzoic acid, 2-methylbenzenesulfonamide and phosphorousoxychloride 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 then filtered, dried and recrystallized from methanol (m.p. 450 K). Colourless prismatic crystals were obtained by slow evaporation of a solution of the title compound in methanol (with a few drops of water).

## Refinement

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{14}H_{12}INO_3S$ |
| $M_r$ | 401.21 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 173 |
| $a, b, c$ (Å) | 11.0543 (10), 12.1612 (10), 12.3464 (10) |
| $\alpha, \beta, \gamma$ (°) | 119.140 (4), 94.668 (5), 93.182 (5) |
| $V$ (Å$^3$) | 1436.2 (2) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 18.94 |
| Crystal size (mm) | 0.25 × 0.12 × 0.07 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2009) |
| $T_{min}$, $T_{max}$ | 0.124, 0.266 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 17365, 4724, 3621 |
| $R_{int}$ | 0.092 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.585 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.062, 0.182, 1.05 |
| No. of reflections | 4724 |
| No. of parameters | 363 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.40, −1.39 |

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

## Acknowledgements

The authors are thankful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, Mysore, for providing the single-crystal X-ray diffraction data.

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# full crystallographic data

*IUCrData* (2017). **2**, x162030 [https://doi.org/10.1107/S2414314616020307]

## 4-Iodo-*N*-(*o*-tolylsulfonyl)benzamide

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### 4-Iodo-*N*-(*o*-tolylsulfonyl)benzamide

*Crystal data*

$C_{14}H_{12}INO_3S$
$M_r$ = 401.21
Triclinic, $P\overline{1}$
$a$ = 11.0543 (10) Å
$b$ = 12.1612 (10) Å
$c$ = 12.3464 (10) Å
$\alpha$ = 119.140 (4)°
$\beta$ = 94.668 (5)°
$\gamma$ = 93.182 (5)°
$V$ = 1436.2 (2) Å$^3$
$Z$ = 4
$F(000)$ = 784
$D_x$ = 1.855 Mg m$^{-3}$
Melting point: 450 K
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 133 reflections
$\theta$ = 4.0–64.4°
$\mu$ = 18.94 mm$^{-1}$
$T$ = 173 K
Prism, colourless
0.25 × 0.12 × 0.07 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: sealed X-ray tube
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
$T_{min}$ = 0.124, $T_{max}$ = 0.266
17365 measured reflections
4724 independent reflections
3621 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.092
$\theta_{max}$ = 64.4°, $\theta_{min}$ = 5.4°
$h$ = −12→12
$k$ = −14→14
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.182
$S$ = 1.05
4724 reflections
363 parameters
0 restraints
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.113P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.39 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 | 0.99795 (6) | 0.28147 (5) | −0.25297 (5) | 0.0394 (2) |
| S1 | 0.7516 (2) | 0.17454 (18) | 0.35284 (17) | 0.0273 (5) |
| O1 | 0.8316 (6) | 0.1073 (5) | 0.3869 (5) | 0.0318 (13) |
| O2 | 0.7190 (6) | 0.2922 (5) | 0.4501 (5) | 0.0321 (14) |
| O3 | 0.8181 (6) | 0.0118 (5) | 0.1084 (5) | 0.0330 (14) |
| N1 | 0.8113 (7) | 0.2141 (6) | 0.2560 (6) | 0.0269 (15) |
| H1 | 0.827821 | 0.294813 | 0.279541 | 0.032* |
| C1 | 0.6178 (8) | 0.0717 (7) | 0.2660 (7) | 0.0297 (19) |
| C2 | 0.5212 (9) | 0.1108 (8) | 0.2142 (8) | 0.033 (2) |
| C3 | 0.4173 (10) | 0.0220 (9) | 0.1534 (9) | 0.042 (2) |
| H3 | 0.350362 | 0.043818 | 0.117099 | 0.051* |
| C4 | 0.4096 (9) | −0.0963 (8) | 0.1449 (9) | 0.039 (2) |
| H4 | 0.337588 | −0.153414 | 0.103983 | 0.047* |
| C5 | 0.5066 (9) | −0.1317 (8) | 0.1958 (8) | 0.038 (2) |
| H5 | 0.502342 | −0.213616 | 0.187899 | 0.045* |
| C6 | 0.6086 (8) | −0.0465 (7) | 0.2577 (7) | 0.0304 (19) |
| H6 | 0.673931 | −0.068811 | 0.295485 | 0.036* |
| C7 | 0.8359 (8) | 0.1234 (7) | 0.1386 (7) | 0.0256 (18) |
| C8 | 0.8786 (8) | 0.1684 (7) | 0.0545 (7) | 0.0258 (17) |
| C9 | 0.8854 (8) | 0.2944 (8) | 0.0827 (7) | 0.0289 (19) |
| H9 | 0.865884 | 0.357746 | 0.161014 | 0.035* |
| C10 | 0.9214 (9) | 0.3274 (8) | −0.0055 (7) | 0.032 (2) |
| H10 | 0.926372 | 0.413321 | 0.013469 | 0.039* |
| C11 | 0.9497 (9) | 0.2338 (8) | −0.1213 (7) | 0.0316 (19) |
| C12 | 0.9445 (8) | 0.1084 (8) | −0.1473 (7) | 0.0310 (19) |
| H12 | 0.965631 | 0.044622 | −0.224612 | 0.037* |
| C13 | 0.9083 (8) | 0.0768 (8) | −0.0598 (7) | 0.0314 (19) |
| H13 | 0.903828 | −0.009000 | −0.078578 | 0.038* |
| C14 | 0.5249 (10) | 0.2348 (9) | 0.2182 (9) | 0.044 (2) |
| H14A | 0.446169 | 0.241537 | 0.180359 | 0.066* |
| H14B | 0.589802 | 0.241554 | 0.171524 | 0.066* |
| H14C | 0.541018 | 0.303192 | 0.305187 | 0.066* |
| I2 | 0.35056 (6) | 0.47630 (6) | −0.11241 (5) | 0.0407 (2) |
| S2 | 0.1444 (2) | 0.40351 (17) | 0.52510 (17) | 0.0275 (5) |
| O4 | 0.1960 (6) | 0.5154 (5) | 0.6401 (5) | 0.0320 (14) |
| O5 | 0.0172 (6) | 0.3659 (5) | 0.5076 (5) | 0.0355 (14) |
| O6 | 0.1204 (6) | 0.2389 (5) | 0.2576 (5) | 0.0338 (14) |
| N2 | 0.1819 (6) | 0.4363 (6) | 0.4157 (6) | 0.0268 (15) |
| H2 | 0.212606 | 0.513728 | 0.437907 | 0.032* |
| C15 | 0.2244 (9) | 0.2757 (7) | 0.5050 (6) | 0.0288 (19) |
| C16 | 0.3543 (9) | 0.2878 (8) | 0.5247 (7) | 0.034 (2) |
| C17 | 0.4071 (10) | 0.1809 (9) | 0.5084 (8) | 0.041 (2) |
| H17 | 0.493510 | 0.185113 | 0.521427 | 0.049* |
| C18 | 0.3371 (10) | 0.0675 (9) | 0.4733 (8) | 0.041 (2) |
| H18 | 0.376524 | −0.004767 | 0.459878 | 0.049* |

| | | | | |
|---|---|---|---|---|
| C19 | 0.2115 (9) | 0.0583 (8) | 0.4578 (7) | 0.035 (2) |
| H19 | 0.164404 | −0.018055 | 0.438802 | 0.042* |
| C20 | 0.1550 (9) | 0.1618 (7) | 0.4703 (7) | 0.032 (2) |
| H20 | 0.068594 | 0.155170 | 0.455117 | 0.038* |
| C21 | 0.1661 (8) | 0.3449 (8) | 0.2899 (7) | 0.0278 (18) |
| C22 | 0.2132 (8) | 0.3842 (8) | 0.2011 (7) | 0.0288 (18) |
| C23 | 0.2159 (9) | 0.2872 (8) | 0.0803 (7) | 0.034 (2) |
| H23 | 0.189032 | 0.202605 | 0.058519 | 0.041* |
| C24 | 0.2564 (9) | 0.3118 (8) | −0.0073 (8) | 0.035 (2) |
| H24 | 0.260178 | 0.244419 | −0.089385 | 0.042* |
| C25 | 0.2927 (9) | 0.4363 (9) | 0.0234 (8) | 0.038 (2) |
| C26 | 0.2897 (9) | 0.5353 (8) | 0.1443 (7) | 0.033 (2) |
| H26 | 0.314058 | 0.620255 | 0.165411 | 0.040* |
| C27 | 0.2505 (9) | 0.5079 (7) | 0.2332 (7) | 0.031 (2) |
| H27 | 0.249286 | 0.574251 | 0.316386 | 0.038* |
| C28 | 0.4340 (10) | 0.4063 (8) | 0.5610 (9) | 0.041 (2) |
| H28A | 0.431842 | 0.466625 | 0.649623 | 0.062* |
| H28B | 0.404602 | 0.443550 | 0.510389 | 0.062* |
| H28C | 0.518041 | 0.386688 | 0.546863 | 0.062* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I1 | 0.0546 (5) | 0.0361 (4) | 0.0307 (3) | −0.0023 (3) | 0.0084 (3) | 0.0191 (2) |
| S1 | 0.0345 (12) | 0.0241 (10) | 0.0250 (9) | 0.0008 (8) | 0.0023 (8) | 0.0140 (7) |
| O1 | 0.039 (4) | 0.031 (3) | 0.030 (3) | 0.002 (3) | −0.002 (2) | 0.020 (2) |
| O2 | 0.046 (4) | 0.026 (3) | 0.024 (3) | −0.004 (3) | 0.008 (2) | 0.013 (2) |
| O3 | 0.040 (4) | 0.027 (3) | 0.036 (3) | 0.007 (3) | 0.010 (3) | 0.018 (2) |
| N1 | 0.036 (4) | 0.025 (3) | 0.024 (3) | 0.002 (3) | 0.004 (3) | 0.016 (3) |
| C1 | 0.039 (6) | 0.025 (4) | 0.023 (4) | 0.002 (4) | 0.000 (3) | 0.011 (3) |
| C2 | 0.035 (5) | 0.030 (4) | 0.034 (4) | 0.005 (4) | 0.000 (4) | 0.015 (3) |
| C3 | 0.039 (6) | 0.039 (5) | 0.046 (5) | 0.002 (4) | −0.004 (4) | 0.021 (4) |
| C4 | 0.030 (5) | 0.033 (5) | 0.044 (5) | 0.000 (4) | −0.002 (4) | 0.012 (4) |
| C5 | 0.041 (6) | 0.026 (4) | 0.040 (5) | −0.001 (4) | −0.001 (4) | 0.013 (4) |
| C6 | 0.031 (5) | 0.031 (4) | 0.030 (4) | 0.003 (4) | 0.005 (3) | 0.015 (3) |
| C7 | 0.024 (5) | 0.019 (4) | 0.033 (4) | −0.003 (3) | 0.000 (3) | 0.014 (3) |
| C8 | 0.027 (5) | 0.024 (4) | 0.029 (4) | 0.006 (3) | 0.003 (3) | 0.015 (3) |
| C9 | 0.031 (5) | 0.029 (4) | 0.024 (4) | 0.002 (4) | 0.005 (3) | 0.011 (3) |
| C10 | 0.050 (6) | 0.024 (4) | 0.024 (4) | −0.004 (4) | 0.004 (4) | 0.013 (3) |
| C11 | 0.041 (6) | 0.028 (4) | 0.028 (4) | 0.008 (4) | 0.005 (4) | 0.015 (3) |
| C12 | 0.041 (6) | 0.028 (4) | 0.023 (4) | 0.012 (4) | 0.001 (3) | 0.011 (3) |
| C13 | 0.037 (5) | 0.024 (4) | 0.033 (4) | 0.002 (4) | 0.003 (4) | 0.013 (3) |
| C14 | 0.054 (7) | 0.033 (5) | 0.047 (5) | 0.001 (4) | −0.012 (5) | 0.024 (4) |
| I2 | 0.0423 (4) | 0.0562 (4) | 0.0381 (3) | 0.0068 (3) | 0.0069 (3) | 0.0340 (3) |
| S2 | 0.0382 (13) | 0.0222 (9) | 0.0259 (9) | 0.0050 (8) | 0.0072 (8) | 0.0142 (7) |
| O4 | 0.053 (4) | 0.019 (3) | 0.025 (3) | −0.001 (3) | 0.011 (3) | 0.011 (2) |
| O5 | 0.041 (4) | 0.029 (3) | 0.041 (3) | 0.001 (3) | 0.009 (3) | 0.020 (2) |
| O6 | 0.048 (4) | 0.021 (3) | 0.031 (3) | 0.001 (3) | 0.001 (3) | 0.013 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.031 (4) | 0.024 (3) | 0.032 (3) | 0.002 (3) | 0.006 (3) | 0.019 (3) |
| C15 | 0.047 (6) | 0.026 (4) | 0.017 (3) | 0.007 (4) | 0.006 (3) | 0.012 (3) |
| C16 | 0.046 (6) | 0.038 (5) | 0.030 (4) | 0.011 (4) | 0.014 (4) | 0.024 (4) |
| C17 | 0.052 (7) | 0.045 (5) | 0.034 (4) | 0.016 (5) | 0.009 (4) | 0.024 (4) |
| C18 | 0.054 (7) | 0.037 (5) | 0.044 (5) | 0.019 (5) | 0.012 (4) | 0.028 (4) |
| C19 | 0.053 (7) | 0.023 (4) | 0.033 (4) | 0.003 (4) | 0.002 (4) | 0.017 (3) |
| C20 | 0.047 (6) | 0.026 (4) | 0.027 (4) | −0.003 (4) | −0.001 (4) | 0.018 (3) |
| C21 | 0.029 (5) | 0.025 (4) | 0.029 (4) | 0.005 (4) | 0.002 (3) | 0.012 (3) |
| C22 | 0.032 (5) | 0.029 (4) | 0.029 (4) | 0.000 (4) | −0.001 (3) | 0.018 (3) |
| C23 | 0.047 (6) | 0.029 (4) | 0.028 (4) | 0.006 (4) | 0.003 (4) | 0.014 (3) |
| C24 | 0.049 (6) | 0.034 (5) | 0.031 (4) | 0.010 (4) | 0.007 (4) | 0.022 (4) |
| C25 | 0.041 (6) | 0.052 (6) | 0.033 (4) | 0.007 (4) | −0.002 (4) | 0.029 (4) |
| C26 | 0.039 (6) | 0.032 (4) | 0.032 (4) | −0.003 (4) | 0.003 (4) | 0.020 (4) |
| C27 | 0.046 (6) | 0.026 (4) | 0.023 (4) | 0.005 (4) | 0.005 (4) | 0.012 (3) |
| C28 | 0.044 (6) | 0.036 (5) | 0.051 (5) | 0.002 (4) | 0.002 (4) | 0.028 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| I1—C11 | 2.071 (8) | I2—C25 | 2.095 (9) |
| S1—O1 | 1.408 (6) | S2—O5 | 1.420 (7) |
| S1—O2 | 1.440 (6) | S2—O4 | 1.447 (6) |
| S1—N1 | 1.659 (7) | S2—N2 | 1.659 (6) |
| S1—C1 | 1.770 (9) | S2—C15 | 1.753 (8) |
| O3—C7 | 1.219 (9) | O6—C21 | 1.213 (10) |
| N1—C7 | 1.390 (10) | N2—C21 | 1.389 (10) |
| N1—H1 | 0.8800 | N2—H2 | 0.8800 |
| C1—C6 | 1.388 (11) | C15—C20 | 1.393 (12) |
| C1—C2 | 1.419 (12) | C15—C16 | 1.424 (13) |
| C2—C3 | 1.407 (13) | C16—C17 | 1.385 (13) |
| C2—C14 | 1.483 (12) | C16—C28 | 1.490 (13) |
| C3—C4 | 1.387 (13) | C17—C18 | 1.390 (14) |
| C3—H3 | 0.9500 | C17—H17 | 0.9500 |
| C4—C5 | 1.392 (13) | C18—C19 | 1.376 (14) |
| C4—H4 | 0.9500 | C18—H18 | 0.9500 |
| C5—C6 | 1.375 (13) | C19—C20 | 1.383 (12) |
| C5—H5 | 0.9500 | C19—H19 | 0.9500 |
| C6—H6 | 0.9500 | C20—H20 | 0.9500 |
| C7—C8 | 1.485 (11) | C21—C22 | 1.509 (11) |
| C8—C13 | 1.387 (11) | C22—C23 | 1.383 (12) |
| C8—C9 | 1.392 (12) | C22—C27 | 1.384 (12) |
| C9—C10 | 1.409 (11) | C23—C24 | 1.357 (12) |
| C9—H9 | 0.9500 | C23—H23 | 0.9500 |
| C10—C11 | 1.401 (12) | C24—C25 | 1.395 (13) |
| C10—H10 | 0.9500 | C24—H24 | 0.9500 |
| C11—C12 | 1.395 (12) | C25—C26 | 1.393 (13) |
| C12—C13 | 1.390 (12) | C26—C27 | 1.386 (12) |
| C12—H12 | 0.9500 | C26—H26 | 0.9500 |
| C13—H13 | 0.9500 | C27—H27 | 0.9500 |

| | | | |
|---|---|---|---|
| C14—H14A | 0.9800 | C28—H28A | 0.9800 |
| C14—H14B | 0.9800 | C28—H28B | 0.9800 |
| C14—H14C | 0.9800 | C28—H28C | 0.9800 |
| | | | |
| O1—S1—O2 | 118.2 (3) | O5—S2—O4 | 118.4 (4) |
| O1—S1—N1 | 110.5 (4) | O5—S2—N2 | 110.8 (4) |
| O2—S1—N1 | 103.9 (3) | O4—S2—N2 | 103.2 (3) |
| O1—S1—C1 | 108.4 (4) | O5—S2—C15 | 109.0 (4) |
| O2—S1—C1 | 109.7 (4) | O4—S2—C15 | 109.2 (4) |
| N1—S1—C1 | 105.3 (4) | N2—S2—C15 | 105.4 (4) |
| C7—N1—S1 | 121.8 (5) | C21—N2—S2 | 121.8 (6) |
| C7—N1—H1 | 119.1 | C21—N2—H2 | 119.1 |
| S1—N1—H1 | 119.1 | S2—N2—H2 | 119.1 |
| C6—C1—C2 | 121.5 (8) | C20—C15—C16 | 121.3 (8) |
| C6—C1—S1 | 116.5 (6) | C20—C15—S2 | 117.0 (7) |
| C2—C1—S1 | 121.8 (6) | C16—C15—S2 | 121.7 (6) |
| C3—C2—C1 | 115.9 (8) | C17—C16—C15 | 116.4 (8) |
| C3—C2—C14 | 119.5 (8) | C17—C16—C28 | 119.5 (9) |
| C1—C2—C14 | 124.6 (8) | C15—C16—C28 | 124.1 (8) |
| C4—C3—C2 | 122.1 (9) | C16—C17—C18 | 121.8 (10) |
| C4—C3—H3 | 119.0 | C16—C17—H17 | 119.1 |
| C2—C3—H3 | 119.0 | C18—C17—H17 | 119.1 |
| C3—C4—C5 | 120.4 (9) | C19—C18—C17 | 121.1 (8) |
| C3—C4—H4 | 119.8 | C19—C18—H18 | 119.5 |
| C5—C4—H4 | 119.8 | C17—C18—H18 | 119.5 |
| C6—C5—C4 | 119.0 (9) | C18—C19—C20 | 119.0 (8) |
| C6—C5—H5 | 120.5 | C18—C19—H19 | 120.5 |
| C4—C5—H5 | 120.5 | C20—C19—H19 | 120.5 |
| C5—C6—C1 | 121.1 (9) | C19—C20—C15 | 120.3 (9) |
| C5—C6—H6 | 119.5 | C19—C20—H20 | 119.9 |
| C1—C6—H6 | 119.5 | C15—C20—H20 | 119.9 |
| O3—C7—N1 | 118.9 (7) | O6—C21—N2 | 119.8 (7) |
| O3—C7—C8 | 123.4 (7) | O6—C21—C22 | 123.6 (7) |
| N1—C7—C8 | 117.6 (6) | N2—C21—C22 | 116.5 (7) |
| C13—C8—C9 | 119.6 (7) | C23—C22—C27 | 120.0 (8) |
| C13—C8—C7 | 116.7 (7) | C23—C22—C21 | 115.7 (7) |
| C9—C8—C7 | 123.6 (7) | C27—C22—C21 | 124.3 (7) |
| C8—C9—C10 | 119.7 (7) | C24—C23—C22 | 120.6 (8) |
| C8—C9—H9 | 120.2 | C24—C23—H23 | 119.7 |
| C10—C9—H9 | 120.2 | C22—C23—H23 | 119.7 |
| C11—C10—C9 | 120.2 (7) | C23—C24—C25 | 119.9 (8) |
| C11—C10—H10 | 119.9 | C23—C24—H24 | 120.1 |
| C9—C10—H10 | 119.9 | C25—C24—H24 | 120.1 |
| C12—C11—C10 | 119.5 (8) | C26—C25—C24 | 120.3 (8) |
| C12—C11—I1 | 120.3 (6) | C26—C25—I2 | 119.4 (7) |
| C10—C11—I1 | 120.2 (6) | C24—C25—I2 | 120.3 (6) |
| C13—C12—C11 | 119.8 (7) | C27—C26—C25 | 118.9 (8) |
| C13—C12—H12 | 120.1 | C27—C26—H26 | 120.5 |

| | | | |
|---|---|---|---|
| C11—C12—H12 | 120.1 | C25—C26—H26 | 120.5 |
| C8—C13—C12 | 121.2 (8) | C22—C27—C26 | 120.2 (7) |
| C8—C13—H13 | 119.4 | C22—C27—H27 | 119.9 |
| C12—C13—H13 | 119.4 | C26—C27—H27 | 119.9 |
| C2—C14—H14A | 109.5 | C16—C28—H28A | 109.5 |
| C2—C14—H14B | 109.5 | C16—C28—H28B | 109.5 |
| H14A—C14—H14B | 109.5 | H28A—C28—H28B | 109.5 |
| C2—C14—H14C | 109.5 | C16—C28—H28C | 109.5 |
| H14A—C14—H14C | 109.5 | H28A—C28—H28C | 109.5 |
| H14B—C14—H14C | 109.5 | H28B—C28—H28C | 109.5 |
| | | | |
| O1—S1—N1—C7 | 63.1 (7) | O5—S2—N2—C21 | −62.5 (7) |
| O2—S1—N1—C7 | −169.1 (6) | O4—S2—N2—C21 | 169.7 (7) |
| C1—S1—N1—C7 | −53.8 (7) | C15—S2—N2—C21 | 55.2 (8) |
| O1—S1—C1—C6 | 6.3 (7) | O5—S2—C15—C20 | 3.3 (7) |
| O2—S1—C1—C6 | −124.1 (6) | O4—S2—C15—C20 | 134.0 (6) |
| N1—S1—C1—C6 | 124.6 (6) | N2—S2—C15—C20 | −115.7 (6) |
| O1—S1—C1—C2 | −177.6 (6) | O5—S2—C15—C16 | −176.0 (6) |
| O2—S1—C1—C2 | 52.0 (8) | O4—S2—C15—C16 | −45.2 (7) |
| N1—S1—C1—C2 | −59.3 (8) | N2—S2—C15—C16 | 65.0 (7) |
| C6—C1—C2—C3 | −0.6 (12) | C20—C15—C16—C17 | −0.5 (11) |
| S1—C1—C2—C3 | −176.5 (7) | S2—C15—C16—C17 | 178.8 (6) |
| C6—C1—C2—C14 | −179.3 (8) | C20—C15—C16—C28 | 179.5 (8) |
| S1—C1—C2—C14 | 4.8 (12) | S2—C15—C16—C28 | −1.2 (11) |
| C1—C2—C3—C4 | 0.1 (14) | C15—C16—C17—C18 | 0.7 (12) |
| C14—C2—C3—C4 | 178.9 (9) | C28—C16—C17—C18 | −179.3 (8) |
| C2—C3—C4—C5 | −0.7 (15) | C16—C17—C18—C19 | −2.4 (13) |
| C3—C4—C5—C6 | 1.8 (14) | C17—C18—C19—C20 | 3.8 (13) |
| C4—C5—C6—C1 | −2.4 (13) | C18—C19—C20—C15 | −3.6 (12) |
| C2—C1—C6—C5 | 1.8 (12) | C16—C15—C20—C19 | 2.0 (11) |
| S1—C1—C6—C5 | 177.9 (7) | S2—C15—C20—C19 | −177.3 (6) |
| S1—N1—C7—O3 | −3.3 (11) | S2—N2—C21—O6 | 2.3 (12) |
| S1—N1—C7—C8 | 174.6 (6) | S2—N2—C21—C22 | −175.2 (6) |
| O3—C7—C8—C13 | −5.3 (13) | O6—C21—C22—C23 | −8.0 (13) |
| N1—C7—C8—C13 | 177.0 (8) | N2—C21—C22—C23 | 169.4 (8) |
| O3—C7—C8—C9 | 172.1 (8) | O6—C21—C22—C27 | 171.0 (9) |
| N1—C7—C8—C9 | −5.6 (12) | N2—C21—C22—C27 | −11.6 (13) |
| C13—C8—C9—C10 | 0.5 (13) | C27—C22—C23—C24 | 0.9 (14) |
| C7—C8—C9—C10 | −176.8 (8) | C21—C22—C23—C24 | 180.0 (9) |
| C8—C9—C10—C11 | 0.2 (14) | C22—C23—C24—C25 | −1.8 (15) |
| C9—C10—C11—C12 | −1.3 (14) | C23—C24—C25—C26 | 1.3 (15) |
| C9—C10—C11—I1 | 178.3 (7) | C23—C24—C25—I2 | −178.2 (7) |
| C10—C11—C12—C13 | 1.6 (14) | C24—C25—C26—C27 | 0.2 (14) |
| I1—C11—C12—C13 | −178.0 (7) | I2—C25—C26—C27 | 179.6 (7) |
| C9—C8—C13—C12 | −0.2 (13) | C23—C22—C27—C26 | 0.6 (14) |
| C7—C8—C13—C12 | 177.4 (8) | C21—C22—C27—C26 | −178.4 (8) |
| C11—C12—C13—C8 | −0.9 (14) | C25—C26—C27—C22 | −1.1 (14) |

*Hydrogen-bond geometry (Å, º)*

Cg is the centroid of the iodobenzene ring (C8–C13) of molecule *A*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.88 | 2.06 | 2.900 (10) | 158 |
| N2—H2···O2$^{i}$ | 0.88 | 2.12 | 2.970 (10) | 161 |
| C9—H9···O4$^{i}$ | 0.95 | 2.36 | 3.301 (10) | 170 |
| C13—H13···O6$^{ii}$ | 0.95 | 2.56 | 3.378 (11) | 144 |
| C23—H23···O3$^{ii}$ | 0.95 | 2.40 | 3.201 (11) | 142 |
| C27—H27···O2$^{i}$ | 0.95 | 2.51 | 3.428 (9) | 163 |
| C4—H4···*Cg*$^{iii}$ | 0.93 | 2.81 | 3.656 (11) | 151 |

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