

# Crystal structure and Hirshfeld surface analysis of a halogen bond between 2-(allylthio)pyridine and 1,2,4,5-tetrafluoro-3,6-diiodobenzene

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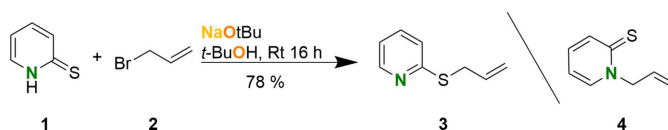
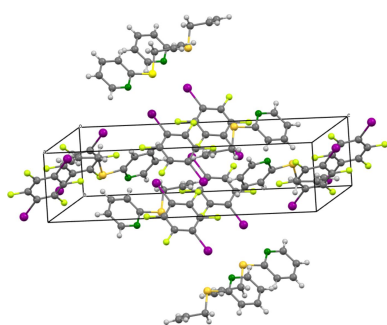
The crystal structure of the title 2:1 molecular complex between 2-(allylthio)pyridine and 1,2,4,5-tetrafluoro-3,6-diiodobenzene,  $C_6F_4I_2 \cdot 2C_8H_9NS$ , at 100 K has been determined in the monoclinic space group  $P2_1/c$ . The most noteworthy characteristic of the complex is the halogen bond between iodine and the pyridine ring with a short  $N \cdots I$  contact [2.8628 (12) Å]. The Hirshfeld surface analysis shows that the hydrogen  $\cdots$  hydrogen contacts dominate the crystal packing with a contribution of 32.1%.

## 1. Chemical context

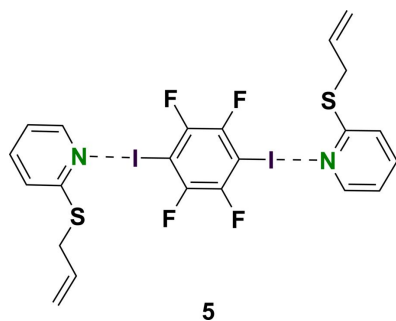
Earlier research investigated the deprotonation of allylic silicon compounds with organolithium reagents (Strohmann *et al.*, 2006). In this work, 2-(allylthio)pyridine was synthesized to compare the chemical behavior to similar systems. The chosen synthetic route was adapted from the literature (Baudin *et al.*, 1993) and could lead to two similar products (Fig. 1) that would be hard to distinguish based on  $^1H$ - and  $^{13}C$ -NMR alone. Since the 2-(allylthio)pyridine did not crystallize and was quite impure, 1,2,4,5-tetrafluoro-3,6-diiodobenzene was added, which led to a two-component co-crystal referred to as complex **5**. Halogen bonds between an aromatic iodine compound and a nitrogen compound can vary in their bond strength, length and angle (Otte *et al.*, 2023). Since only the desired compound formed a halogen bond, the product could be separated from the impurities by simply isolating the co-crystals. Afterwards the 2-(allylthio)pyridine was reobtained by column chromatography.

## 2. Structural commentary

Complex **5** crystallized from heptane at 193.15 K as colorless plates in the monoclinic space group  $P2_1/c$ . The asymmetric unit consists of one molecule of **3** and half a molecule of 1,2,4,5-tetrafluoro-3,6-diiodobenzene. The second half is generated by inversion symmetry (Fig. 2; symmetry operation  $-x, -y, 1 - z$ ). The formula unit of the title compound consists of two molecules 2-(allylthio)pyridine and one molecule 1,2,4,5-tetrafluoro-3,6-diiodobenzene, which lies on an inversion center.

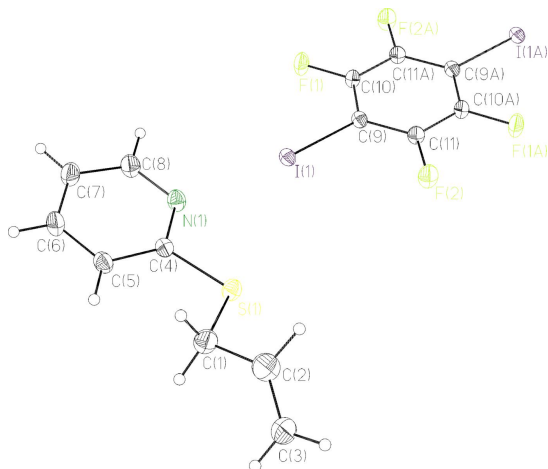


**Figure 1**  
Synthesis of 2-(allylthio)pyridine **3** or 1-allylpyridine-2(1H)-thione **4**.



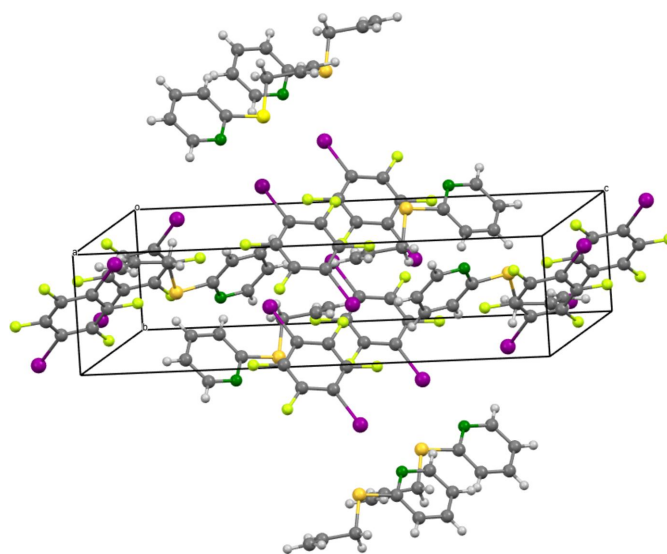
The complex consists of multiple functional groups: an allyl group, a thioether, a pyridine and a perfluorinated diiodobenzene. The C1–C2 bond length [1.492 (2) Å] is longer than the C2–C3 bond length [1.316 (3) Å], which is explained by the double bond between C2 and C3. These lengths coincide with the C–C single bond length of 1.54 Å in ethane and the C=C double bond length of 1.33 Å in ethene (Lide, 2005). The C4–S1–C1 bond angle [102.91 (7)°] is a little bit larger than the C–S–C angle in dimethylsulfide [99.2 (1)°; Mitzel & Losehand, 2004]. The difference in bond angles might be explained by the larger pyridine substituent, of which C4 is a part. The bond lengths in the pyridine ring [C4–C5: 1.3976 (18) Å, C5–C6: 1.391 (2) Å, C6–C7: 1.387 (2) Å, C7–C8: 1.384 (2) Å, C8–N1: 1.3454 (18) Å and N1–C4: 1.3422 (17) Å] are not significantly longer compared to the bond lengths in pyridine (Lide, 2005). The bond angles of the pyridine moiety vary around 118°, which is typical for pyridine. The largest deviations from planarity of the pyridine (r.m.s. deviation 0.010 Å) are observed for C7 [−0.0124 (12) Å] and C4 [−0.0140 (9) Å]. The angle between the normal of the pyridine plane (N1,C4–C8) and the double bond between C2 and C3 is 115.35 (13)°.

The bond lengths and angles of 1,2,4,5,-tetrafluoro-3,6-diiodobenzene are consistent with those present in the Cambridge Structural Database. The benzene ring makes a dihedral angle of 12.88 (5)° with the pyridine ring.



**Figure 2**

The molecular structure of the title compound **5**, showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

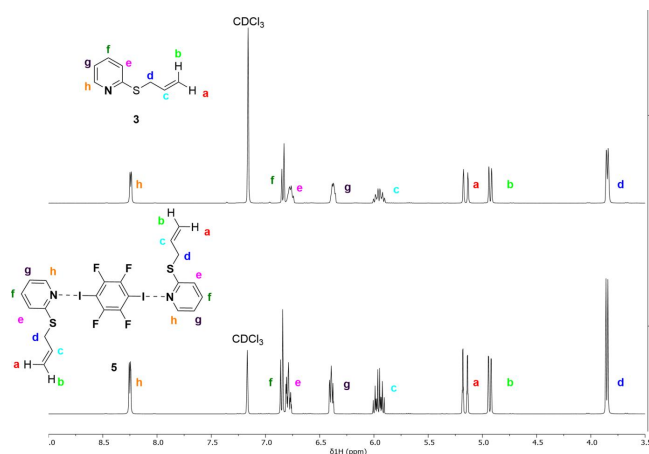


**Figure 3**

A view of the packing of **5**.

### 3. Supramolecular features

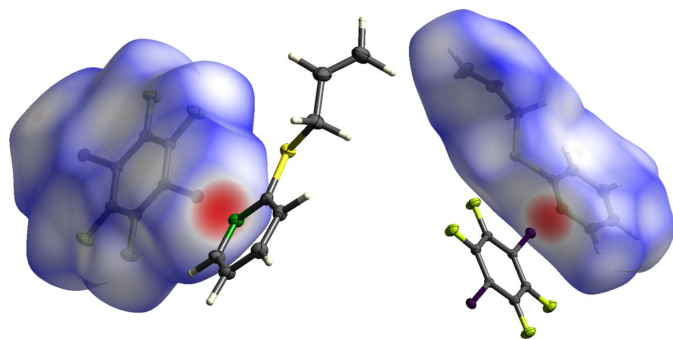
Fig. 3 shows the packing of the complex. The most important supramolecular feature is the close contact between N1 and I1 with a coordination distance of 2.8628 (12) Å, which is shorter than the sum of the van der Waals radii of 3.73 Å (Nyburg & Faerman, 1985). The strength of a halogen bond is determined by the bond length and the bond angle. Strong halogen bonds are expected to have a bond length in the region of 2.781 (2) Å (Otte *et al.*, 2023), which is shorter than the distance observed for **5**. The N1–I1–C9 bond angle is 173.90 (4)°, which is slightly less than a theoretical ideal angle of 180°. In conclusion, the here presented structure shows a medium-strength halogen bond between N1 and I1. Further evidence for this is the small difference in <sup>1</sup>H-NMR chemical shifts between compounds **3** and **5** (Fig. 4). Theoretically, the sulfur present here could also form a halogen bond with the iodine, but this behavior is not observed.



**Figure 2**  
<sup>1</sup>H-NMR of compound **3** and **5**

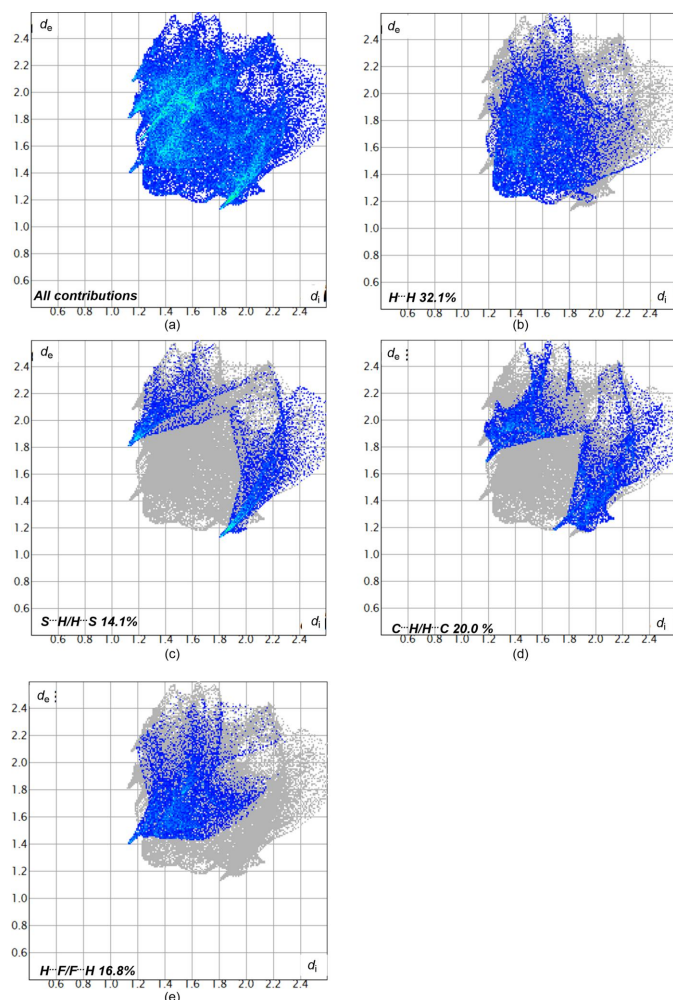
**Figure 4**

<sup>1</sup>H-NMR spectra (400 MHz) of compounds **3** and **5** in CDCl<sub>3</sub>.



**Figure 5**  
Three-dimensional Hirshfeld surface of **5** mapped over  $d_{\text{norm}}$ .

To better understand the van der Waals interactions, a Hirshfeld surface analysis was performed. In Fig. 5, the Hirshfeld surface generated by *CrystalExplorer21* (Spackman *et al.*, 2021) is mapped over  $d_{\text{norm}}$  (Spackman & Jayatilaka, 2009) and red dots are used to represent close contacts.



**Figure 6**  
Two-dimensional fingerprint plots for **5** showing (a) all interactions, and (b)–(e) delineated into contributions from other contacts (blue areas) [ $d_e$  and  $d_i$  represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

For further exploration of the intermolecular interactions, two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were generated as shown in Fig. 6. The H...H interaction with a contribution of 32.1% has the biggest impact on the packing in the solid state. The C...H/H...C bonds with 20.0%, F...H with 16.8%, S...H/H...S with 14.1%, N...H/H...N with 3.3%, N...I/I...N with 3.2% C...I/I...C with 2.2% or N...C/C...N with 1.5% are less impactful in comparison.

#### 4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.45, last update June 2024; Groom *et al.*, 2016) for 1,2,4,5-tetrafluoro-3,6-diiodobenzene yielded 802 hits. In 261 structures, the iodo atom interacts with a pyridine nitrogen atom with N...I distances ranging from 2.662 to 3.511 Å and averaging 2.911 Å. The mean C—I...N angle is 171.9°.

A search for the keywords halogen bond, thioether and pyridine leads to a structure of 1,2,4,5-tetrafluoro-3,6-diiodobenzene-4-(pyridin-4-ylsulfanyl)pyridine (1/1) (Arman *et al.*, 2010). The variety of publications containing halogen bonds is quite large and includes the previously discussed strong halogen bond with quinuclidine (Otte *et al.*, 2023) or halogen bonds with carbonyl hypiodites as bond donors (Yu *et al.*, 2021). The structural motif of thioethers is also well known, especially in the context of ligand chemistry with silicon-based thioethers for palladium (Schneider *et al.*, 2023; Bastero *et al.*, 2002) or silver (Nomiya *et al.*, 1996; Gaudillat *et al.*, 2023). Sulfonium-based ionic liquids (Zhao *et al.*, 2007) and other systems like (*Z*)-3-allyl-5-(4-nitrobenzylidene)-2-sulfanylidene-1,3-thiazolidin-4-one (Moreno *et al.*, 2024) are good examples of compounds with allyl groups.

#### 5. Synthesis and crystallization

Complex **5** was synthesized by adding 1,2,4,5-tetrafluoro-3,6-diiodobenzene (293.96 g mol<sup>-1</sup>, 0.33 mmol, 0.5 eq., 97.19 mg) to a solution of 2-(allylthio)pyridine (151.23 g mol<sup>-1</sup>, 0.66 mmol, 1.0 eq., 100.00 mg) and pentane at room temperature. The solution was stirred for one h and crystallized at 193.15 K.

<sup>1</sup>H NMR (400 MHz, benzene-*d*<sub>6</sub>, ppm): 8.24 (*dt*,  $J = 4.9, 1.4$ , 2H, C<sub>5</sub>H<sub>4</sub>N), 6.80 (*ddt*,  $J = 27.0, 6.3, 1.6$ , 4H, C<sub>5</sub>H<sub>4</sub>N), 6.41–6.34 (*m*, 2H, C<sub>5</sub>H<sub>4</sub>N), 5.95 (*ddd*,  $J = 16.9, 10.1, 1.5$ , 2H, CH—CH<sub>2</sub>), 5.15 (*dq*,  $J = 16.9, 1.5$ , 2H, CH—CH<sub>2</sub>), 4.93 (*dt*,  $J = 10.0, 1.3$ , 2H, CH—CH<sub>2</sub>), 3.85 (*dq*,  $J = 6.9, 1.3$ , 4H, S—CH<sub>2</sub>).

<sup>13</sup>C NMR (101 MHz, benzene-*d*<sub>6</sub>, ppm): 159.10 (C<sub>5</sub>H<sub>4</sub>N), 149.60 (C<sub>5</sub>H<sub>4</sub>N), 135.66 (C<sub>6</sub>F<sub>4</sub>I<sub>2</sub>), 134.68 (C<sub>6</sub>F<sub>4</sub>I<sub>2</sub>), 122.28 (C<sub>5</sub>H<sub>4</sub>N), 119.23 (CH—CH<sub>2</sub>), 117.15 (C<sub>5</sub>H<sub>4</sub>N), 65.93 (C<sub>5</sub>H<sub>4</sub>N), 32.88 (CH—CH<sub>2</sub>), 15.60 (C<sub>6</sub>F<sub>4</sub>I<sub>2</sub>), 1.42 (S—CH<sub>2</sub>).

<sup>19</sup>F NMR (377 MHz, benzene-*d*<sub>6</sub>, ppm): −118.86 (C<sub>6</sub>F<sub>4</sub>I<sub>2</sub>).

#### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Hydrogen atoms were positioned geometrically (C—H = 0.95–1.00 Å) and were refined using a

riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for  $\text{CH}_2$  and CH hydrogen atoms.

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**Table 1**

Experimental details.

Crystal data	
Chemical formula	$2\text{C}_8\text{H}_9\text{NS}\cdot\text{C}_6\text{F}_4\text{I}_2$
$M_r$	704.30
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
$a, b, c$ (Å)	11.184 (2), 5.2951 (6), 20.544 (3)
$\beta$ (°)	96.137 (6)
$V$ (Å <sup>3</sup> )	1209.7 (3)
$Z$	2
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	2.82
Crystal size (mm)	0.25 × 0.23 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.468, 0.567
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	91740, 5719, 5342
$R_{\text{int}}$	0.036
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.827
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.019, 0.047, 1.12
No. of reflections	5719
No. of parameters	181
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.91, -0.73

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

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## supporting information

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## Crystal structure and Hirshfeld surface analysis of a halogen bond between 2-(allylthio)pyridine and 1,2,4,5-tetrafluoro-3,6-diiodobenzene

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### Computing details

#### Bis[2-(prop-2-en-1-ylsulfanyl)pyridine] 1,2,4,5-tetrafluoro-3,6-diiodobenzene

##### Crystal data

$2\text{C}_8\text{H}_9\text{NS}\cdot\text{C}_6\text{F}_4\text{I}_2$

$M_r = 704.30$

Monoclinic,  $P2_1/c$

$a = 11.184$  (2) Å

$b = 5.2951$  (6) Å

$c = 20.544$  (3) Å

$\beta = 96.137$  (6)°

$V = 1209.7$  (3) Å<sup>3</sup>

$Z = 2$

$F(000) = 676$

$D_x = 1.934$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 9219 reflections

$\theta = 4.0\text{--}28.0^\circ$

$\mu = 2.82$  mm<sup>-1</sup>

$T = 100$  K

Plate, colourless

$0.25 \times 0.23 \times 0.07$  mm

##### Data collection

Bruker APEXII CCD

diffractometer

Radiation source: microfocus sealed X-ray tube,

Incoatec I $\mu$ s

Mirror optics monochromator

Detector resolution: 7.9 pixels mm<sup>-1</sup>

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.468$ ,  $T_{\max} = 0.567$

91740 measured reflections

5719 independent reflections

5342 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 36.0^\circ$ ,  $\theta_{\min} = 1.8^\circ$

$h = -17 \rightarrow 18$

$k = -8 \rightarrow 8$

$l = -33 \rightarrow 33$

##### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.019$

$wR(F^2) = 0.047$

$S = 1.12$

5719 reflections

181 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0187P)^2 + 0.9301P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.91$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.73$  e Å<sup>-3</sup>

##### 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.13965 (2)	0.45457 (2)	0.60714 (2)	0.01556 (2)
S1	0.40259 (3)	0.94040 (6)	0.63185 (2)	0.02017 (6)
F1	-0.07102 (9)	0.05135 (19)	0.62168 (4)	0.02486 (17)
F2	0.17962 (9)	0.28759 (19)	0.45993 (5)	0.02646 (18)
N1	0.22969 (11)	0.8241 (2)	0.70166 (6)	0.01990 (19)
C10	-0.03525 (12)	0.0315 (2)	0.56133 (6)	0.01663 (19)
C5	0.34960 (12)	1.1694 (3)	0.74802 (7)	0.0211 (2)
C7	0.17783 (15)	1.0299 (3)	0.79911 (7)	0.0245 (3)
C11	0.09192 (11)	0.1455 (2)	0.48116 (6)	0.01691 (19)
C9	0.05773 (11)	0.1819 (2)	0.54352 (6)	0.01517 (18)
C6	0.27543 (14)	1.1910 (3)	0.79795 (7)	0.0248 (3)
C4	0.32194 (11)	0.9853 (2)	0.70003 (6)	0.01659 (19)
C8	0.15980 (14)	0.8479 (3)	0.75070 (7)	0.0236 (2)
C1	0.49191 (14)	1.2265 (3)	0.63106 (8)	0.0259 (3)
C2	0.53357 (17)	1.2510 (4)	0.56476 (9)	0.0324 (3)
C3	0.64683 (17)	1.2469 (5)	0.55287 (9)	0.0376 (4)
H3A	0.666 (3)	1.271 (6)	0.5084 (14)	0.057 (8)*
H8	0.091 (2)	0.735 (5)	0.7506 (12)	0.037 (6)*
H5	0.418 (2)	1.273 (5)	0.7475 (11)	0.035 (6)*
H7	0.126 (2)	1.040 (5)	0.8317 (14)	0.042 (7)*
H1A	0.441 (2)	1.372 (6)	0.6366 (13)	0.042 (7)*
H2	0.463 (2)	1.259 (6)	0.5245 (13)	0.050 (8)*
H6	0.291 (2)	1.313 (5)	0.8299 (11)	0.033 (6)*
H1B	0.564 (2)	1.215 (5)	0.6661 (11)	0.032 (6)*
H3B	0.714 (2)	1.232 (5)	0.5891 (12)	0.039 (7)*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
I1	0.01687 (4)	0.01338 (3)	0.01582 (3)	0.00101 (2)	-0.00106 (2)	-0.00098 (2)
S1	0.02284 (14)	0.01741 (13)	0.02085 (13)	0.00025 (11)	0.00504 (11)	-0.00131 (11)
F1	0.0313 (4)	0.0287 (5)	0.0160 (3)	-0.0073 (4)	0.0087 (3)	-0.0051 (3)
F2	0.0292 (4)	0.0281 (4)	0.0235 (4)	-0.0131 (4)	0.0095 (3)	-0.0036 (3)
N1	0.0244 (5)	0.0172 (5)	0.0182 (4)	-0.0040 (4)	0.0027 (4)	-0.0015 (4)
C10	0.0192 (5)	0.0171 (5)	0.0139 (4)	-0.0002 (4)	0.0031 (4)	-0.0016 (4)
C5	0.0220 (5)	0.0191 (5)	0.0217 (5)	-0.0024 (4)	-0.0004 (4)	-0.0039 (4)
C7	0.0285 (6)	0.0265 (6)	0.0192 (5)	-0.0014 (5)	0.0056 (5)	-0.0027 (5)
C11	0.0185 (5)	0.0162 (5)	0.0163 (5)	-0.0021 (4)	0.0028 (4)	-0.0003 (4)
C9	0.0166 (4)	0.0137 (4)	0.0148 (4)	0.0009 (4)	-0.0001 (3)	-0.0005 (4)
C6	0.0298 (6)	0.0234 (6)	0.0210 (6)	-0.0018 (5)	0.0019 (5)	-0.0066 (5)
C4	0.0180 (5)	0.0148 (5)	0.0165 (5)	0.0008 (4)	-0.0001 (4)	0.0002 (4)
C8	0.0269 (6)	0.0240 (6)	0.0202 (5)	-0.0068 (5)	0.0047 (4)	-0.0017 (5)
C1	0.0276 (6)	0.0232 (6)	0.0281 (7)	-0.0057 (5)	0.0082 (5)	-0.0014 (5)
C2	0.0346 (8)	0.0356 (9)	0.0274 (7)	-0.0067 (7)	0.0047 (6)	0.0066 (6)
C3	0.0336 (8)	0.0541 (12)	0.0263 (7)	-0.0108 (8)	0.0090 (6)	-0.0044 (8)

*Geometric parameters (Å, °)*

I1—N1	2.8628 (12)	C7—C6	1.387 (2)
I1—C9	2.0921 (12)	C7—C8	1.384 (2)
S1—C4	1.7613 (14)	C7—H7	0.94 (3)
S1—C1	1.8158 (16)	C11—C9	1.3891 (17)
F1—C10	1.3471 (15)	C6—H6	0.92 (2)
F2—C11	1.3452 (15)	C8—H8	0.97 (3)
N1—C4	1.3422 (17)	C1—C2	1.492 (2)
N1—C8	1.3454 (18)	C1—H1A	0.97 (3)
C10—C11 <sup>i</sup>	1.3867 (18)	C1—H1B	1.03 (2)
C10—C9	1.3895 (18)	C2—C3	1.316 (3)
C5—C6	1.391 (2)	C2—H2	1.09 (3)
C5—C4	1.3976 (18)	C3—H3A	0.97 (3)
C5—H5	0.94 (3)	C3—H3B	1.01 (2)
C9—I1—N1	173.90 (4)	C7—C6—C5	119.64 (13)
C4—S1—C1	102.91 (7)	C7—C6—H6	120.4 (15)
C4—N1—I1	129.30 (9)	N1—C4—S1	113.22 (10)
C4—N1—C8	117.96 (12)	N1—C4—C5	122.60 (12)
C8—N1—I1	112.43 (9)	C5—C4—S1	124.17 (10)
F1—C10—C11 <sup>i</sup>	118.13 (11)	N1—C8—C7	123.47 (14)
F1—C10—C9	120.12 (11)	N1—C8—H8	117.6 (15)
C11 <sup>i</sup> —C10—C9	121.74 (11)	C7—C8—H8	118.9 (15)
C6—C5—C4	118.22 (13)	S1—C1—H1A	109.2 (16)
C6—C5—H5	120.7 (15)	S1—C1—H1B	109.7 (14)
C4—C5—H5	121.0 (15)	C2—C1—S1	107.84 (12)
C6—C7—H7	122.0 (17)	C2—C1—H1A	106.4 (16)
C8—C7—C6	118.05 (14)	C2—C1—H1B	110.3 (13)
C8—C7—H7	119.9 (17)	H1A—C1—H1B	113 (2)
F2—C11—C10 <sup>i</sup>	118.29 (11)	C1—C2—H2	115.2 (15)
F2—C11—C9	120.24 (11)	C3—C2—C1	124.68 (17)
C10 <sup>i</sup> —C11—C9	121.45 (11)	C3—C2—H2	120.0 (15)
C10—C9—I1	121.41 (9)	C2—C3—H3A	119.0 (17)
C11—C9—I1	121.77 (9)	C2—C3—H3B	121.7 (14)
C11—C9—C10	116.81 (11)	H3A—C3—H3B	119 (2)
C5—C6—H6	120.0 (15)		
I1—N1—C4—S1	-4.91 (15)	C6—C5—C4—S1	177.45 (11)
I1—N1—C4—C5	174.94 (10)	C6—C5—C4—N1	-2.4 (2)
I1—N1—C8—C7	-173.81 (13)	C6—C7—C8—N1	-2.1 (2)
S1—C1—C2—C3	-117.0 (2)	C4—S1—C1—C2	-162.02 (12)
F1—C10—C9—I1	-2.97 (17)	C4—N1—C8—C7	0.3 (2)
F1—C10—C9—C11	178.18 (12)	C4—C5—C6—C7	0.5 (2)
F2—C11—C9—I1	-0.19 (17)	C8—N1—C4—S1	-177.88 (11)
F2—C11—C9—C10	178.65 (12)	C8—N1—C4—C5	2.0 (2)
C10 <sup>i</sup> —C11—C9—I1	-178.42 (10)	C8—C7—C6—C5	1.6 (2)
C10 <sup>i</sup> —C11—C9—C10	0.4 (2)	C1—S1—C4—N1	165.66 (10)

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C11 <sup>i</sup> —C10—C9—I1	178.43 (10)	C1—S1—C4—C5	-14.19 (14)
C11 <sup>i</sup> —C10—C9—C11	-0.4 (2)		

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Symmetry code: (i)  $-x, -y, -z+1$ .