research communications

# Synthesis and crystal structure of (E)-1,2-bis[2-(methylsulfanyl)phenyl]diazene

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The title compound, $C_{14}H_{14}N_2S_2$, was obtained by transmetallation of 2,2′-bis(trimethylstannyl)azobenzene with methyl lithium, and subsequent quenching with dimethyl disulfide. The asymmetric unit comprises two half-molecules, the other halves being completed by inversion symmetry at the midpoint of the azo group. The two molecules show only slight differences with respect to N=N, S—N and aromatic C=C bonds or angles. Hirshfeld surface analysis reveals that except for one weak H···S interaction, intermolecular interactions are dominated by van der Waals forces only.

1. Chemical context

The molecular switch azobenzene can undergo isomerization from its thermodynamically stable *trans* form to the meta-stable *cis* form using external stimuli such as light, temperature or pressure. Azobenzenes are common motifs in dyes because of their high thermal and photochemical stability (Yesodha *et al.*, 2004; Lagrasta *et al.*, 1997). We recently presented methods to substitute azobenzenes in the *ortho*, *meta* and *para*-positions with trimethyltin as a novel functionalization method, giving rise to a dual tin–lithium exchange (Strüben *et al.*, 2014, 2015; Hoffmann *et al.*, 2019). In particular, we described the effect on the di*ortho*-substitution on azobenzenes with trimethyl-tetrels and the resulting effects on the switching properties (Hoffmann *et al.*, 2019). In this context, we present here a novel di*ortho*-substituted azobenzene, $(C_7H_7NS)_2$, (I), bearing two methylsulfide groups.
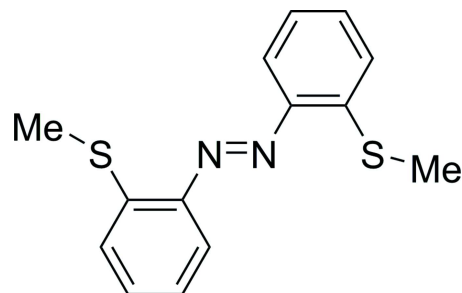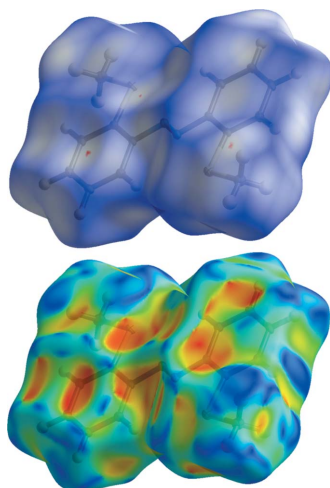
2. Structural commentary

The asymmetric unit of the title compound consists of two half-molecules (**Ia** and **Ib**), the other halves being completed by application of inversion symmetry. The midpoints of the N=N bonds are located on inversion centres, resulting in a
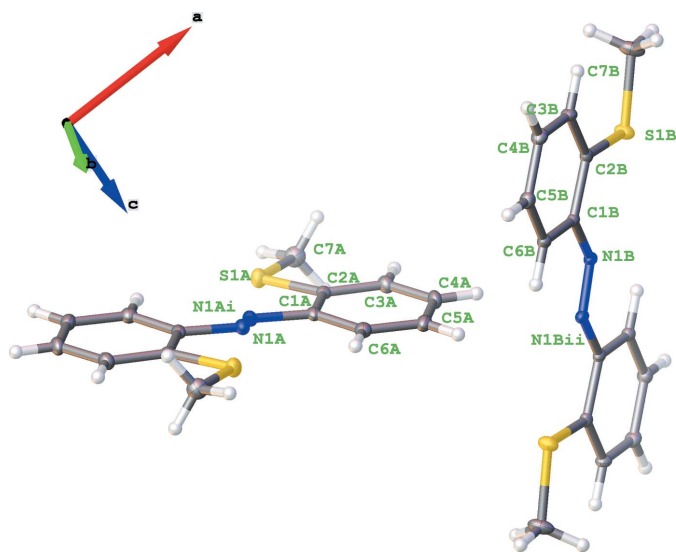
Figure 1
Molecular structures (**Ia** left, **Ib** right) of the title compound with labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) x, $1 - y$, $- z$; (ii) $1 - x$, $1 - y$, $1 - z$.]

Figure 3
Crystal packing in a view along the b axis. To distinguish the different molecules, all sulfur atoms within the unit cell are labelled.

trans-configuration for the central N=N bonds (Fig. 1). As indicated by the C6A—C1A—N1A—N1A^i and C6B—C1B—N1B—N1B^{ii} [symmetry codes: (i) $-x$, $1 - y$, $-z$; (ii) $1 - x$, $1 - y$, $1 - z$] torsion angles of 13.2 (2) and −5.3 (2)°, respectively, in both molecules the phenyl rings are twisted slightly with respect to the azo unit. A weak distortion is also found for the N1—C1—C2—S1 torsion angles of −3.06 (16)° for **Ia** and −2.06 (15)° for **Ib**. The N=N bond lengths differ marginally [1.255 (2) Å for **Ia**, 1.264 (2) Å for **Ib**], as do comparable C—C bonds. For example, the C1—C2 bond in **Ia** is at 1.408 (2) Å slightly shorter than **Ib** [1.415 (2) Å]. In comparison, this bond is longer than all other C—C distances in the ring because of repulsion of the nitrogen and the sulfur atoms attached to C1 and C2, respectively. In both molecules, the S···N distances [2.8625 (13) Å for **Ia**, 2.8761 (11) Å for **Ib**] are too long to be considered as attractive interactions. Fig. 2 represents an overlay plot of the two molecules, showing there are only slight conformational differences.

3. Supramolecular features and Hirshfeld surface analysis

The packing of **Ia** and **Ib** in the crystal is shown in Fig. 3. Despite the presence of phenyl rings and a parallel arrange-

ment of the molecules, only weak offset π–π interactions are observed; the shortest centroid-to-centroid distance is $Cg2\cdots Cg2(1 - x, 1 - y, -z) = 3.7525$ (8) Å with a slippage of 1.422 Å. To further investigate the intermolecular interactions, Hirshfeld surfaces (Hirshfeld, 1977) and fingerprint plots were generated for both molecules using *CrystalExplorer17.5*

Figure 4
Hirshfeld surface of **Ia** mapped with d_{norm} (top) and shape index (bottom), displaying no significant intermolecular interactions.

Figure 2
Overlay presentation of molecules **Ia** and **Ib**.

Figure 5
Hirshfeld surface of **Ib** mapped with d_{norm} (top) and shape index (bottom) with indication of an S···H interaction.

(McKinnon *et al.*, 2004). Hirshfeld surface analysis depicts intermolecular interactions by different colors, representing s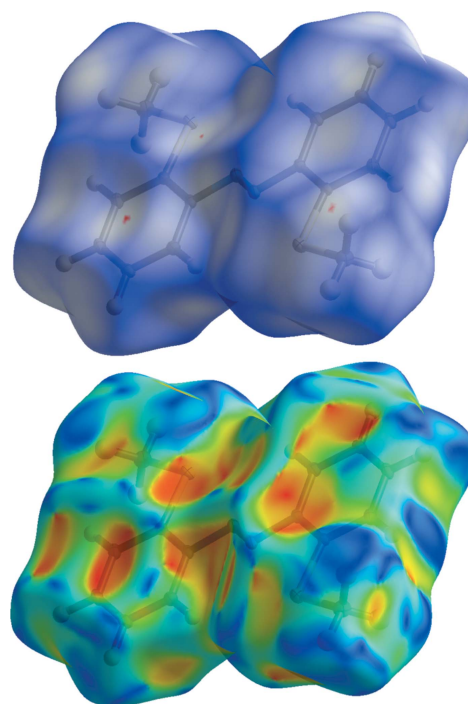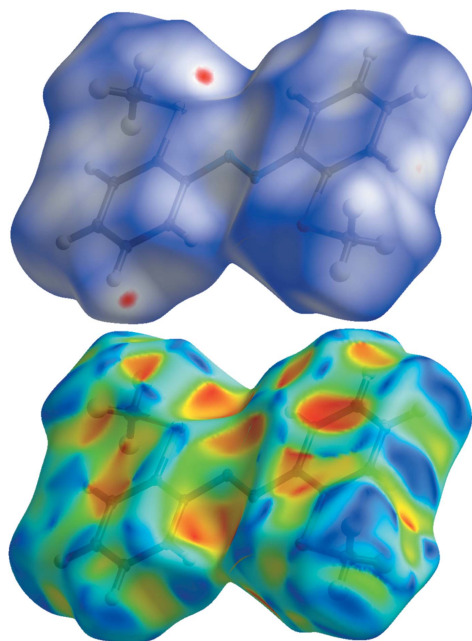hort or long contacts and further the relative strength of the interaction. The generated Hirshfeld surfaces mapped over d_{norm} and the shape index are shown in Fig. 4 for **Ia** and in Fig. 5 for **Ib**. Whereas in **Ia** a significant intermolecular interaction is not apparent, characteristic red spots near S1*B* and H5*B* indicate weak S···H interactions in **Ib**. The respective supramolecular arrangement is shown in Fig. 6. The sulfur atom S1*B* interacts with a phenyl proton (H4*B*) of another molecule of **Ib** (S···H distance = 2.811 Å). The two-dimensional fingerprint plots for molecule **Ib** for quantification of the contributions of each type of non-covalent interaction to the Hirshfeld surface (McKinnon *et al.*, 2007) are given in Fig. 7. The packing is dominated by H···H contacts, representing van der Waals interactions (44.5% contribution to the surface), followed by C···H and S···H interactions, which contribute with 24.0% and 18.1%, respectively. The contri-
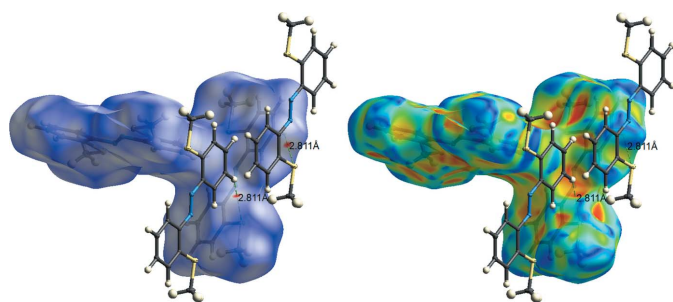

Figure 6
Hirshfeld surface of **Ib** mapped with d_{norm} (left) and shape index (right), together with the interaction of a neighbouring molecule.
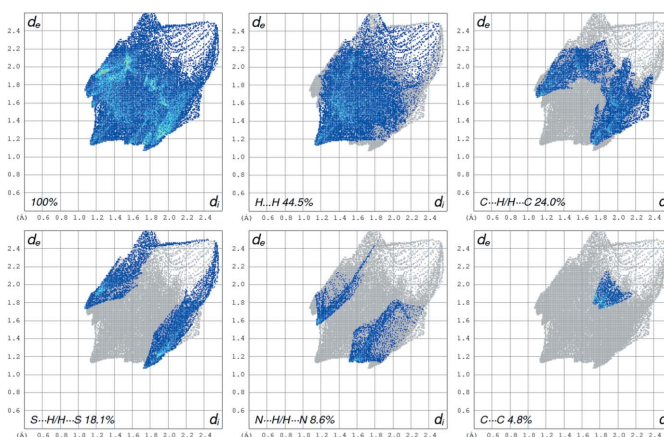

Figure 7
Two-dimensional fingerprint plots for **Ib**, delineated into H···H, C···H, S···H, N···H, C···C interactions.

butions of the N···H (8.6%) and C···C (4.8%) interactions are less significant.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.4.0; update August 2019; Groom *et al.*, 2016) revealed no azobenzene-based structures that contain methyl thioethers. However, some general *ortho*-substituted azobenzenes have been deposited (Yamamura *et al.*, 2008; Kano *et al.*, 2001; Hoffmann *et al.*, 2019). Additionally, some di*ortho*-substituted thioazoxybenzenes were reported previously (Szczygelska-Tao *et al.*, 1999; Kertmen *et al.*, 2013). For the structure of an azobenzene compound with an inversion centre at the N=N bond, see: Bohle *et al.* (2007).

5. Synthesis and crystallization

The synthesis of 2,2′-*bis*(trimethylstannyl)azobenzene was recently described (Hoffmann *et al.*, 2019). For further details of a similar transmetallation of a stannylated azobenzene, see: Strüben *et al.* (2015). Dimethyl disulfide (99%) was purchased from Acros Organics and was used without further purification. Methyl lithium (1.88 *M* in diethyl ether, titrated against 2,2′-bipyridine) was purchased from Acros Organics. THF was purchased from VWR and was dried and degassed with a solvent purification system by Inert Technology.

2,2′-*bis*(Methylthio)azobenzene

In an inert reaction tube, 2,2-*bis*(trimethylstannyl)azo-stannyl)azobenzene (200 mg, 0.39 mmol) was dissolved under Schlenk conditions in THF (12.5 ml) and cooled to 195 K. Then MeLi (1.88 *M* in diethyl ether, 0.63 ml, 1.18 mmol) was added within 5 min and after 1.5 h at this temperature, dimethyl disulfide (0.35 ml, 3.94 mmol) was added in one ration. The reaction mixture was warmed to 298 K over 14 h and the solvent was removed under reduced pressure. The obtained orange solid was purified in a silica column (Merck, 0.015–0.40 mm) with a gradient of eluents from *n*-pentane to

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}N_2S_2$
M_r	274.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.0656 (5), 12.1787 (4), 8.3471 (3)
β (°)	96.154 (1)
V (Å^3)	1320.55 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.39
Crystal size (mm)	$0.21 \times 0.18 \times 0.17$
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.580, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21000, 3292, 2842
R_{int}	0.065
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.089, 1.04
No. of reflections	3292
No. of parameters	165
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.44, −0.38

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

dichloromethane giving dark-orange crystals (31 mg, 0.11 mmol; yield 29%). Single crystals suitable for X-ray analysis were obtained by slow evaporation from a saturated *n*-heptane solution.

^{1}H NMR (500 MHz, CDCl$_3$): δ = 7.76 (*dd*, ^3J = 8.1 Hz, ^4J = 1.4 Hz, 2H, *H*6), 7.40 (*td*, ^3J = 8.0, 7.3 Hz, ^4J = 1.4 Hz, 2H, *H*4), 7.32 (*dd*, ^3J = 8.0 Hz, ^4J = 1.1 Hz, 2H, *H*3), 7.20 (*td*, ^3J = 8.1, 7.3Hz, ^4J = 1.1 Hz, 2H, *H*5), 2.53 (*s*, 6H, *H*7) ppm.

^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$): δ = 149.08 (*C*1), 141.00 (*C*2), 131.56 (*C*4), 124.81 (*C*3), 124.75 (*C*5), 118.02 (*C*6), 15.02 (*C*7) ppm.

HRMS (EI, 70 eV, MAT95, direct): *m/z*: calculated for $C_{14}H_{14}N_2S_2^+$ 274.05929 found 274.05944.

MS (EI): *m/z* 273.9 (5%) [*M*]$^+$, 258.9 (100%) [*M* − CH$_3$]$^+$, 243.9 (5%) [*M* − C$_2$H$_6$]$^+$, 107.9 (13%) [*M* − C$_8$H$_{10}$N$_2$S]$^+$.

IR (ATR): ν = 3059 (*w*), 2986 (*w*), 2961 (*w*), 2918 (*w*), 2852 (*w*), 1575 (*m*), 1561 (*w*), 1457 (*m*), 1433 (*s*), 1298 (*w*), 1249 (*w*), 1217 (*m*), 1162 (*m*), 1065 (*s*), 1035 (*m*), 951 (*m*), 863 (*w*), 803 (*w*), 761 (*s*), 726 (*s*), 674 (*s*) cm^{-1}.

M.p.: 429 K

R_f: (*n*-pentane: dichloromethane 3:1): 0.55.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were positioned geometrically and refined using a riding model: C—H = 0.95–0.98 Å with U_{iso}(H) = 1.5U_{eq} (C-methyl) and 1.2U_{eq}(C) (C-phenyl).

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supporting information

Synthesis and crystal structure of (*E*)-1,2-bis[2-(methylsulfanyl)phenyl]diazene

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

(*E*)-1,2-Bis[2-(methylsulfanyl)phenyl]diazene

Crystal data

$C_{14}H_{14}N_2S_2$	$F(000) = 576$
$M_r = 274.39$	$D_x = 1.380$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 13.0656$ (5) Å	Cell parameters from 9874 reflections
$b = 12.1787$ (4) Å	$\theta = 2.3–28.3°$
$c = 8.3471$ (3) Å	$\mu = 0.39$ mm^{-1}
$\beta = 96.154$ (1)°	$T = 100$ K
$V = 1320.55$ (8) Å^3	Block, dark orange
$Z = 4$	$0.21 \times 0.18 \times 0.17$ mm

Data collection

Bruker D8 Venture CMOS diffractometer	$T_{min} = 0.580$, $T_{max} = 0.746$
	21000 measured reflections
Radiation source: microfocus sealed X-ray tube, Incoatec Iμs	3292 independent reflections
	2842 reflections with $I > 2\sigma(I)$
Mirror optics monochromator	$R_{int} = 0.065$
Detector resolution: 7.9 pixels mm^{-1}	$\theta_{max} = 28.3°$, $\theta_{min} = 2.3°$
ω and φ scans	$h = -17 \rightarrow 17$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$k = -16 \rightarrow 16$
	$l = -11 \rightarrow 10$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.6716P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3292 reflections	$(\Delta/\sigma)_{max} < 0.001$
165 parameters	$\Delta\rho_{max} = 0.44$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: dual	

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}
S1A	0.03738 (3)	0.22038 (3)	0.07109 (4)	0.01750 (10)
N1A	0.00557 (9)	0.45111 (10)	0.02308 (14)	0.0144 (2)
C1A	0.09596 (10)	0.43239 (11)	0.13020 (16)	0.0133 (3)
C2A	0.12139 (10)	0.32133 (11)	0.15962 (16)	0.0136 (3)
C3A	0.21227 (10)	0.29785 (12)	0.25937 (17)	0.0163 (3)
H3A	0.232873	0.223733	0.278065	0.020*
C4A	0.27191 (10)	0.38209 (12)	0.33050 (17)	0.0175 (3)
H4A	0.333363	0.364884	0.397179	0.021*
C5A	0.24372 (10)	0.49160 (12)	0.30637 (17)	0.0170 (3)
H5A	0.284385	0.548538	0.358432	0.020*
C6A	0.15556 (10)	0.51642 (12)	0.20540 (16)	0.0153 (3)
H6A	0.135717	0.590824	0.187411	0.018*
C7A	0.09736 (12)	0.09607 (12)	0.15119 (19)	0.0212 (3)
H7AA	0.108296	0.100874	0.268985	0.032*
H7AB	0.163749	0.086347	0.108405	0.032*
H7AC	0.052690	0.033332	0.119805	0.032*
S1B	0.68646 (3)	0.36826 (3)	0.29648 (4)	0.01522 (10)
N1B	0.53057 (8)	0.47643 (9)	0.45728 (13)	0.0111 (2)
C1B	0.54712 (9)	0.53356 (10)	0.31394 (15)	0.0107 (2)
C2B	0.62096 (9)	0.48706 (11)	0.22188 (15)	0.0109 (2)
C3B	0.63884 (10)	0.53770 (11)	0.07713 (16)	0.0135 (3)
H3B	0.688084	0.507481	0.013715	0.016*
C4B	0.58521 (10)	0.63170 (11)	0.02550 (16)	0.0149 (3)
H4B	0.597271	0.664586	−0.073966	0.018*
C5B	0.51371 (10)	0.67861 (11)	0.11794 (16)	0.0141 (3)
H5B	0.478373	0.743923	0.082900	0.017*
C6B	0.49478 (10)	0.62917 (11)	0.26090 (16)	0.0121 (3)
H6B	0.445749	0.660464	0.323699	0.015*
C7B	0.77056 (12)	0.33890 (13)	0.1449 (2)	0.0230 (3)
H7BA	0.729477	0.327171	0.041043	0.035*
H7BB	0.810613	0.272618	0.174984	0.035*
H7BC	0.817418	0.400922	0.136102	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.01446 (17)	0.01894 (19)	0.01851 (19)	−0.00155 (13)	−0.00094 (13)	−0.00187 (13)
N1A	0.0110 (5)	0.0196 (6)	0.0125 (5)	0.0009 (4)	0.0008 (4)	−0.0003 (4)
C1A	0.0098 (6)	0.0203 (7)	0.0100 (6)	−0.0002 (5)	0.0022 (5)	0.0005 (5)

C2A	0.0102 (6)	0.0199 (7)	0.0111 (6)	−0.0010 (5)	0.0032 (5)	−0.0020 (5)
C3A	0.0129 (6)	0.0205 (7)	0.0155 (7)	0.0018 (5)	0.0011 (5)	0.0019 (5)
C4A	0.0112 (6)	0.0267 (7)	0.0139 (6)	0.0008 (5)	−0.0013 (5)	0.0017 (6)
C5A	0.0136 (6)	0.0250 (7)	0.0124 (6)	−0.0033 (5)	0.0013 (5)	−0.0021 (5)
C6A	0.0141 (6)	0.0194 (7)	0.0128 (6)	−0.0005 (5)	0.0029 (5)	0.0000 (5)
C7A	0.0238 (7)	0.0182 (7)	0.0215 (7)	−0.0003 (6)	0.0026 (6)	0.0015 (6)
S1B	0.01542 (17)	0.01406 (17)	0.01718 (18)	0.00275 (12)	0.00642 (13)	0.00248 (12)
N1B	0.0103 (5)	0.0140 (5)	0.0090 (5)	−0.0019 (4)	0.0012 (4)	−0.0012 (4)
C1B	0.0097 (5)	0.0135 (6)	0.0088 (6)	−0.0028 (5)	0.0008 (5)	−0.0014 (5)
C2B	0.0096 (5)	0.0112 (6)	0.0115 (6)	−0.0013 (5)	0.0001 (5)	−0.0013 (5)
C3B	0.0124 (6)	0.0176 (6)	0.0111 (6)	−0.0014 (5)	0.0042 (5)	−0.0018 (5)
C4B	0.0160 (6)	0.0180 (7)	0.0108 (6)	−0.0030 (5)	0.0020 (5)	0.0019 (5)
C5B	0.0142 (6)	0.0146 (6)	0.0130 (6)	0.0002 (5)	0.0000 (5)	0.0011 (5)
C6B	0.0109 (6)	0.0148 (6)	0.0106 (6)	−0.0011 (5)	0.0011 (5)	−0.0020 (5)
C7B	0.0229 (7)	0.0210 (7)	0.0276 (8)	0.0061 (6)	0.0144 (6)	0.0013 (6)

Geometric parameters (Å, º)

S1A—C2A	1.7574 (14)	S1B—C2B	1.7605 (13)
S1A—C7A	1.8002 (15)	S1B—C7B	1.7983 (15)
N1A—N1A[i]	1.255 (2)	N1B—N1B[ii]	1.264 (2)
N1A—C1A	1.4211 (17)	N1B—C1B	1.4205 (16)
C1A—C2A	1.4080 (19)	C1B—C2B	1.4145 (18)
C1A—C6A	1.3940 (19)	C1B—C6B	1.3981 (18)
C2A—C3A	1.4046 (18)	C2B—C3B	1.3983 (18)
C3A—H3A	0.9500	C3B—H3B	0.9500
C3A—C4A	1.383 (2)	C3B—C4B	1.3866 (19)
C4A—H4A	0.9500	C4B—H4B	0.9500
C4A—C5A	1.393 (2)	C4B—C5B	1.3961 (19)
C5A—H5A	0.9500	C5B—H5B	0.9500
C5A—C6A	1.3857 (19)	C5B—C6B	1.3824 (19)
C6A—H6A	0.9500	C6B—H6B	0.9500
C7A—H7AA	0.9800	C7B—H7BA	0.9800
C7A—H7AB	0.9800	C7B—H7BB	0.9800
C7A—H7AC	0.9800	C7B—H7BC	0.9800
C2A—S1A—C7A	101.82 (7)	C2B—S1B—C7B	103.00 (7)
N1A[i]—N1A—C1A	113.98 (14)	N1B[ii]—N1B—C1B	114.53 (14)
C2A—C1A—N1A	115.37 (12)	C2B—C1B—N1B	115.83 (11)
C6A—C1A—N1A	123.50 (13)	C6B—C1B—N1B	124.14 (11)
C6A—C1A—C2A	121.11 (12)	C6B—C1B—C2B	120.02 (12)
C1A—C2A—S1A	118.27 (10)	C1B—C2B—S1B	118.09 (10)
C3A—C2A—S1A	123.84 (11)	C3B—C2B—S1B	123.24 (10)
C3A—C2A—C1A	117.89 (12)	C3B—C2B—C1B	118.67 (12)
C2A—C3A—H3A	119.8	C2B—C3B—H3B	119.8
C4A—C3A—C2A	120.33 (13)	C4B—C3B—C2B	120.46 (12)
C4A—C3A—H3A	119.8	C4B—C3B—H3B	119.8
C3A—C4A—H4A	119.3	C3B—C4B—H4B	119.6

C3A—C4A—C5A	121.35 (13)	C3B—C4B—C5B	120.79 (12)
C5A—C4A—H4A	119.3	C5B—C4B—H4B	119.6
C4A—C5A—H5A	120.4	C4B—C5B—H5B	120.3
C6A—C5A—C4A	119.12 (13)	C6B—C5B—C4B	119.42 (13)
C6A—C5A—H5A	120.4	C6B—C5B—H5B	120.3
C1A—C6A—H6A	119.9	C1B—C6B—H6B	119.7
C5A—C6A—C1A	120.10 (13)	C5B—C6B—C1B	120.63 (12)
C5A—C6A—H6A	119.9	C5B—C6B—H6B	119.7
S1A—C7A—H7AA	109.5	S1B—C7B—H7BA	109.5
S1A—C7A—H7AB	109.5	S1B—C7B—H7BB	109.5
S1A—C7A—H7AC	109.5	S1B—C7B—H7BC	109.5
H7AA—C7A—H7AB	109.5	H7BA—C7B—H7BB	109.5
H7AA—C7A—H7AC	109.5	H7BA—C7B—H7BC	109.5
H7AB—C7A—H7AC	109.5	H7BB—C7B—H7BC	109.5
S1A—C2A—C3A—C4A	−177.02 (11)	S1B—C2B—C3B—C4B	−179.51 (10)
N1A^i—N1A—C1A—C2A	−168.19 (14)	N1B^{ii}—N1B—C1B—C2B	175.48 (13)
N1A^i—N1A—C1A—C6A	13.2 (2)	N1B^{ii}—N1B—C1B—C6B	−5.3 (2)
N1A—C1A—C2A—S1A	−3.06 (16)	N1B—C1B—C2B—S1B	−2.06 (15)
N1A—C1A—C2A—C3A	177.45 (12)	N1B—C1B—C2B—C3B	178.30 (11)
N1A—C1A—C6A—C5A	−178.94 (12)	N1B—C1B—C6B—C5B	−178.56 (12)
C1A—C2A—C3A—C4A	2.4 (2)	C1B—C2B—C3B—C4B	0.11 (19)
C2A—C1A—C6A—C5A	2.5 (2)	C2B—C1B—C6B—C5B	0.61 (19)
C2A—C3A—C4A—C5A	0.3 (2)	C2B—C3B—C4B—C5B	1.1 (2)
C3A—C4A—C5A—C6A	−1.8 (2)	C3B—C4B—C5B—C6B	−1.4 (2)
C4A—C5A—C6A—C1A	0.4 (2)	C4B—C5B—C6B—C1B	0.54 (19)
C6A—C1A—C2A—S1A	175.63 (10)	C6B—C1B—C2B—S1B	178.71 (10)
C6A—C1A—C2A—C3A	−3.86 (19)	C6B—C1B—C2B—C3B	−0.94 (18)
C7A—S1A—C2A—C1A	−176.89 (11)	C7B—S1B—C2B—C1B	−179.91 (10)
C7A—S1A—C2A—C3A	2.57 (13)	C7B—S1B—C2B—C3B	−0.28 (13)

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