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S-Diethylamino-*S*-(3-methylbenzoylimino)-*S*,*S*-diphenylsulfonium tetrafluoroborate

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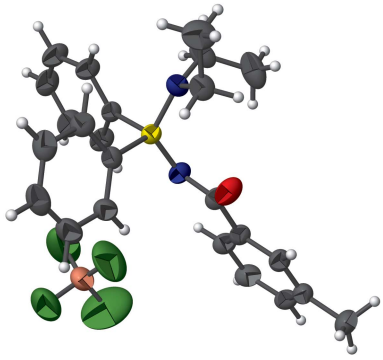
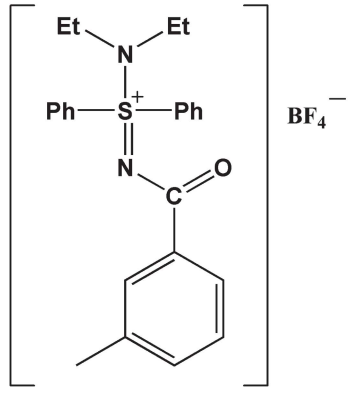
Structural data: full structural data are available from iucrdata.iucr.org

The title salt, $C_{24}H_{27}N_2OS^+\cdot BF_4^-$, was prepared by an alkylation at the amino N atom attached to the sulfur atom of the corresponding sulfodiimide. The configuration around the sulfur atom is a slightly distorted tetrahedral geometry with two S—N bonds and two S—C bonds. The lengths of the S—N(diethylamine) and S═N(*m*-methylbenzoylimine) bonds are 1.619 (2) and 1.551 (2) Å, respectively. The two N—S—N—C(ethyl) and the N—S—N—C(*m*-methylbenzoylimine) torsion angles are −85.43 (3), 58.94 (17) and 62.03 (16)°, respectively. The dihedral angle between the two phenyl rings is 84.03 (14)°. In the crystal, C—H···F hydrogen bonds link the cation and anion, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

The chemistry of sulfur(VI) sulfonium compounds such as oxosulfonium salts is very interesting because of their anomalous reactivity (Mori *et al.*, 1990; Kennewell & Taylor, 1975). However, only a few iminosulfonium salts, which are isoelectronic with the oxosulfonium salts, have been reported (Glemser & Mews, 1980; Labbow *et al.*, 2016). In view of the anomalous reactivity of these salts, we report herein on the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is illustrated in Fig. 1. The S1═N1 (*m*-methylbenzoylimine) and S1—N2 (diethylamine) bond lengths are 1.551 (2) and 1.619 (2) Å, respectively. These bonds are significantly longer than the S≡N triple bond of triphenylsulfanenitrile (1.462 Å; Yoshimura *et al.*, 1997), and close to the S═N double bonds of *S*,*S*-dimethylsulfonediimine (1.533 Å, electron diffraction study; Oberhammer *et al.*, 1970), *S*,*S*-diphenyl-*S*-pyrrolidinoiminosulfonium perchlorate [1.503 (2) Å for S—N

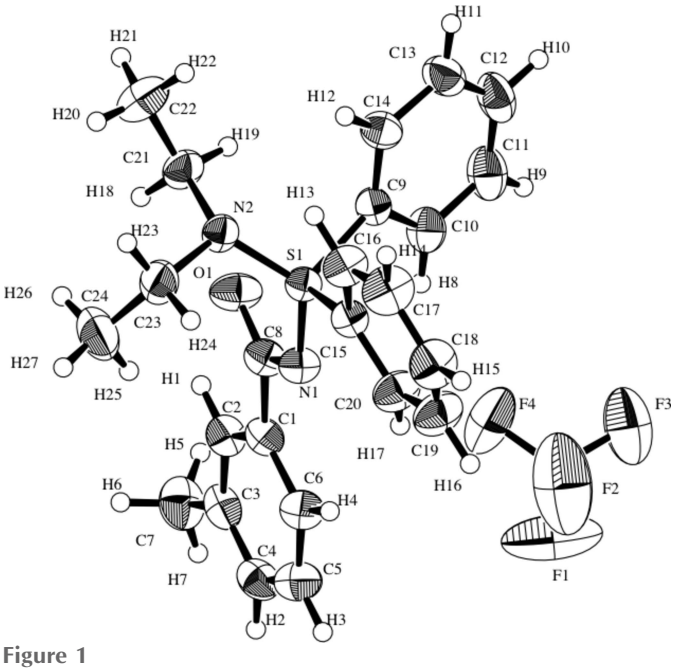


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

(NH), X-ray; Sheikh *et al.*, 2017], sulfonediiminosulfonium salt [1.599 (3) Å for S—N; Ohkubo *et al.*, 1997], *S,S*-diphenyl-*S*-tosyl sulfone diimine [1.515 (18) Å for S—N (NH) and 1.5785 (15) Å for S—N (*p*-toluenesulfonyl), X-ray; Sheikh *et al.*, 2019*b*] and *N*-ethyl-*N*-(3-methylbenzoyl)-*S,S*-diphenylsulfodiimide [1.528 (2) Å for S—N (NEt) and 1.584 (3) Å for S—N (*m*-methylbenzoyl), X-ray; Sheikh *et al.*, 2019*a*], and shorter than that of *S,S*-diphenyl-*N*-tosylsulfilimine (1.628 Å, X-ray; Kálmán *et al.*, 1971). In the crystal, the cation and the anion are linked through weak C—H···F hydrogen bonds (Table 1), forming a three-dimensional network (Fig. 2).

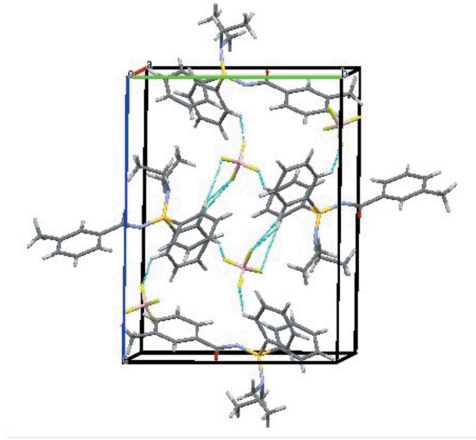


Figure 2
A packing view of the title compound, showing C—H···F hydrogen bonds (blue dashed lines).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H6···F3^{i}	0.98	2.50	3.446 (4)	163
C10—H8···F4	0.95	2.48	3.202 (5)	133
C14—H12···F3^{ii}	0.95	2.51	3.433 (3)	165
C16—H13···F2^{ii}	0.95	2.61	3.367 (4)	137
C16—H13···F3^{ii}	0.95	2.55	3.450 (4)	158
C18—H15···F1^{iii}	0.95	2.33	3.200 (5)	150

Symmetry codes: (i) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{27}N_2OS^+\cdot BF_4^-$
M_r	478.35
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	11.9291 (3), 12.6437 (3), 16.3467 (3)
β (°)	103.5043 (7)
V (Å^3)	2397.36 (8)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	1.64
Crystal size (mm)	0.67 × 0.54 × 0.52
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.256, 0.426
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	26225, 4382, 3856
R_{int}	0.082
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.060, 0.168, 1.05
No. of reflections	4382
No. of parameters	301
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.54, −0.48

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008) and *CrystalStructure* (Rigaku, 2010).

Synthesis and crystallization

The compound precursor, *N*-ethyl-*N*-(3-methylbenzoyl)-*S,S*-diphenylsulfodiimide (363 mg, 1.0 mmol) was allowed to react with triethyloxonium tetrafluoroborate (209 mg, 1.1 mmol) in dry CH_2Cl_2 (30 ml) under argon atmosphere at a temperature of 0°C for 4 h. The reaction mixture was poured into water, and extracted with $CHCl_3$ (3 × 15 ml). The combined organic extracts were washed with water, dried over anhydrous $MgSO_4$. The solution was concentrated under reduced pressure afforded the desired product (yield: 316 mg, 66%) as a colourless solid. Single crystals were obtained from an acetone/ether (2:1 *v*/*v*) solution (m.p. 169.5–170.5°C).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x191040 [https://doi.org/10.1107/S241431461901040X]

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Crystal data

$C_{24}H_{27}N_2OS^+\cdot BF_4^-$
M_r = 478.35
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.9291 (3) Å
b = 12.6437 (3) Å
c = 16.3467 (3) Å
β = 103.5043 (7)°
V = 2397.36 (8) Å^3
Z = 4
$F(000)$ = 1000.00
D_x = 1.325 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 22845 reflections
θ = 3.5–68.3°
μ = 1.64 mm^{-1}
T = 173 K
Prism, colorless
0.67 × 0.54 × 0.52 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.256, T_{max} = 0.426
26225 measured reflections
4382 independent reflections
3856 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.082
θ_{max} = 68.3°
h = −14→14
k = −15→15
l = −19→19

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.168
S = 1.05
4382 reflections
301 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0927P)^2 + 1.2365P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.75784 (4)	0.11353 (4)	0.51723 (3)	0.03166 (19)
F1	0.7005 (3)	−0.0580 (3)	0.8507 (3)	0.1658 (15)
F2	0.6448 (3)	0.1055 (3)	0.80659 (19)	0.1504 (14)
F3	0.8184 (3)	0.0744 (2)	0.88636 (13)	0.1083 (8)
F4	0.7734 (3)	0.0159 (3)	0.75575 (14)	0.1263 (10)
O1	0.86944 (15)	−0.07847 (13)	0.50778 (12)	0.0504 (5)
N1	0.72177 (16)	0.00692 (14)	0.55045 (11)	0.0375 (5)
N2	0.75769 (16)	0.13263 (15)	0.41929 (11)	0.0365 (5)
C1	0.75160 (19)	−0.18041 (17)	0.57664 (13)	0.0371 (5)
C2	0.8086 (2)	−0.27349 (18)	0.56551 (14)	0.0417 (6)
C3	0.7792 (3)	−0.36964 (18)	0.59583 (15)	0.0439 (6)
C4	0.6909 (3)	−0.37093 (19)	0.63708 (16)	0.0470 (6)
C5	0.6343 (3)	−0.2791 (2)	0.64957 (16)	0.0506 (6)
C6	0.6642 (2)	−0.18277 (19)	0.61995 (15)	0.0433 (6)
C7	0.8447 (3)	−0.4689 (2)	0.58432 (18)	0.0607 (8)
C8	0.7884 (2)	−0.08128 (17)	0.54186 (14)	0.0386 (5)
C9	0.89235 (18)	0.16430 (17)	0.57434 (13)	0.0346 (5)
C10	0.9420 (3)	0.11372 (19)	0.64906 (15)	0.0450 (6)
C11	1.0408 (3)	0.1582 (3)	0.69911 (16)	0.0571 (7)
C12	1.0854 (3)	0.2507 (3)	0.67599 (17)	0.0551 (7)
C13	1.0326 (3)	0.3013 (2)	0.60202 (17)	0.0501 (6)
C14	0.9348 (2)	0.25843 (19)	0.54964 (15)	0.0422 (6)
C15	0.65558 (19)	0.20356 (16)	0.53852 (13)	0.0340 (5)
C16	0.6462 (2)	0.30164 (19)	0.49989 (15)	0.0441 (6)
C17	0.5733 (3)	0.3747 (2)	0.52257 (19)	0.0568 (7)
C18	0.5112 (3)	0.3506 (3)	0.58164 (18)	0.0561 (7)
C19	0.5241 (3)	0.2537 (3)	0.62010 (19)	0.0583 (7)
C20	0.5974 (3)	0.1782 (2)	0.59955 (16)	0.0486 (6)
C21	0.8615 (2)	0.1007 (2)	0.38780 (15)	0.0442 (6)
C22	0.8773 (3)	0.1727 (3)	0.31817 (19)	0.0669 (9)
C23	0.6442 (3)	0.1176 (3)	0.35908 (16)	0.0513 (7)
C24	0.6170 (3)	0.0048 (3)	0.3314 (3)	0.0791 (11)
B1	0.7324 (3)	0.0342 (3)	0.82280 (18)	0.0553 (8)
H1	0.8689	−0.2712	0.5365	0.0500*
H2	0.6685	−0.4362	0.6573	0.0564*
H3	0.5742	−0.2820	0.6788	0.0607*
H4	0.6256	−0.1197	0.6291	0.0520*
H5	0.9276	−0.4539	0.5980	0.0729*
H6	0.8206	−0.4927	0.5258	0.0729*
H7	0.8283	−0.5245	0.6217	0.0729*
H8	0.9096	0.0508	0.6655	0.0540*
H9	1.0782	0.1242	0.7500	0.0685*
H10	1.1529	0.2802	0.7111	0.0661*
H11	1.0635	0.3658	0.5870	0.0601*
H12	0.8981	0.2923	0.4985	0.0506*

H13	0.6887	0.3181	0.4591	0.0529*
H14	0.5656	0.4427	0.4972	0.0682*
H15	0.4596	0.4011	0.5955	0.0674*
H16	0.4823	0.2380	0.6614	0.0699*
H17	0.6072	0.1112	0.6266	0.0583*
H18	0.8519	0.0270	0.3669	0.0530*
H19	0.9310	0.1036	0.4347	0.0530*
H20	0.8103	0.1669	0.2705	0.0803*
H21	0.9470	0.1522	0.3001	0.0803*
H22	0.8849	0.2459	0.3384	0.0803*
H23	0.6424	0.1615	0.3086	0.0616*
H24	0.5829	0.1439	0.3856	0.0616*
H25	0.6226	−0.0403	0.3810	0.0949*
H26	0.6720	−0.0196	0.2994	0.0949*
H27	0.5386	0.0010	0.2959	0.0949*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0269 (4)	0.0320 (3)	0.0363 (3)	0.00407 (18)	0.0077 (3)	0.00063 (17)
F1	0.136 (3)	0.150 (3)	0.239 (4)	−0.025 (3)	0.099 (3)	0.069 (3)
F2	0.137 (3)	0.164 (3)	0.117 (2)	0.079 (3)	−0.0370 (18)	−0.0409 (18)
F3	0.1131 (19)	0.1178 (19)	0.0745 (13)	0.0108 (15)	−0.0176 (13)	−0.0239 (13)
F4	0.169 (3)	0.155 (3)	0.0724 (14)	−0.023 (2)	0.0645 (16)	−0.0245 (14)
O1	0.0398 (10)	0.0411 (9)	0.0768 (12)	0.0064 (8)	0.0267 (9)	0.0050 (8)
N1	0.0344 (11)	0.0334 (9)	0.0460 (10)	0.0037 (8)	0.0119 (8)	0.0034 (8)
N2	0.0300 (11)	0.0442 (10)	0.0358 (10)	0.0043 (8)	0.0084 (8)	−0.0016 (8)
C1	0.0322 (13)	0.0346 (11)	0.0416 (12)	0.0019 (9)	0.0028 (9)	0.0009 (9)
C2	0.0403 (14)	0.0384 (12)	0.0449 (12)	0.0039 (10)	0.0071 (10)	−0.0019 (9)
C3	0.0493 (16)	0.0352 (11)	0.0411 (12)	0.0009 (10)	−0.0015 (11)	−0.0018 (9)
C4	0.0498 (16)	0.0385 (12)	0.0468 (13)	−0.0060 (11)	−0.0007 (11)	0.0071 (10)
C5	0.0427 (15)	0.0540 (15)	0.0554 (15)	−0.0018 (12)	0.0119 (12)	0.0100 (12)
C6	0.0366 (14)	0.0422 (12)	0.0502 (13)	0.0039 (10)	0.0083 (10)	0.0051 (10)
C7	0.082 (3)	0.0374 (13)	0.0606 (16)	0.0068 (13)	0.0114 (15)	−0.0022 (11)
C8	0.0308 (13)	0.0363 (11)	0.0479 (12)	0.0037 (10)	0.0076 (10)	0.0005 (10)
C9	0.0270 (12)	0.0387 (11)	0.0375 (11)	0.0049 (9)	0.0062 (9)	−0.0046 (9)
C10	0.0457 (15)	0.0469 (13)	0.0393 (12)	0.0078 (11)	0.0037 (11)	0.0011 (10)
C11	0.0537 (17)	0.0652 (17)	0.0438 (13)	0.0101 (14)	−0.0059 (12)	−0.0045 (12)
C12	0.0353 (15)	0.0698 (17)	0.0541 (15)	0.0023 (13)	−0.0022 (11)	−0.0213 (13)
C13	0.0371 (14)	0.0526 (14)	0.0613 (15)	−0.0059 (12)	0.0133 (12)	−0.0128 (12)
C14	0.0338 (13)	0.0449 (12)	0.0474 (13)	−0.0001 (10)	0.0084 (10)	0.0007 (10)
C15	0.0274 (12)	0.0348 (11)	0.0391 (11)	0.0064 (9)	0.0063 (9)	−0.0020 (8)
C16	0.0416 (14)	0.0417 (12)	0.0502 (13)	0.0111 (11)	0.0135 (11)	0.0063 (10)
C17	0.0575 (18)	0.0437 (14)	0.0709 (18)	0.0203 (12)	0.0184 (14)	0.0080 (12)
C18	0.0508 (17)	0.0512 (15)	0.0692 (17)	0.0179 (13)	0.0196 (14)	−0.0075 (13)
C19	0.0566 (18)	0.0604 (16)	0.0676 (17)	0.0101 (14)	0.0343 (14)	−0.0019 (13)
C20	0.0500 (16)	0.0442 (13)	0.0577 (14)	0.0097 (12)	0.0251 (12)	0.0051 (11)
C21	0.0356 (14)	0.0551 (14)	0.0459 (13)	0.0042 (11)	0.0177 (11)	−0.0033 (10)

C22	0.066 (2)	0.084 (2)	0.0606 (17)	0.0052 (17)	0.0341 (16)	0.0114 (15)
C23	0.0342 (15)	0.0780 (19)	0.0399 (13)	0.0003 (12)	0.0050 (10)	−0.0072 (11)
C24	0.064 (2)	0.099 (3)	0.0704 (19)	−0.0223 (19)	0.0087 (16)	−0.0359 (18)
B1	0.067 (3)	0.0594 (18)	0.0407 (14)	0.0017 (16)	0.0144 (14)	−0.0027 (13)

Geometric parameters (Å, º)

S1—N1	1.551 (2)	C19—C20	1.388 (5)
S1—N2	1.619 (2)	C21—C22	1.503 (5)
S1—C9	1.777 (2)	C23—C24	1.509 (5)
S1—C15	1.762 (3)	C2—H1	0.950
F1—B1	1.339 (6)	C4—H2	0.950
F2—B1	1.358 (5)	C5—H3	0.950
F3—B1	1.375 (4)	C6—H4	0.950
F4—B1	1.320 (5)	C7—H5	0.980
O1—C8	1.224 (4)	C7—H6	0.980
N1—C8	1.395 (3)	C7—H7	0.980
N2—C21	1.503 (4)	C10—H8	0.950
N2—C23	1.488 (3)	C11—H9	0.950
C1—C2	1.392 (4)	C12—H10	0.950
C1—C6	1.391 (4)	C13—H11	0.950
C1—C8	1.484 (4)	C14—H12	0.950
C2—C3	1.388 (4)	C16—H13	0.950
C3—C4	1.377 (5)	C17—H14	0.950
C3—C7	1.513 (4)	C18—H15	0.950
C4—C5	1.382 (4)	C19—H16	0.950
C5—C6	1.388 (4)	C20—H17	0.950
C9—C10	1.383 (3)	C21—H18	0.990
C9—C14	1.390 (4)	C21—H19	0.990
C10—C11	1.387 (4)	C22—H20	0.980
C11—C12	1.374 (5)	C22—H21	0.980
C12—C13	1.383 (4)	C22—H22	0.980
C13—C14	1.386 (4)	C23—H23	0.990
C15—C16	1.384 (4)	C23—H24	0.990
C15—C20	1.380 (4)	C24—H25	0.980
C16—C17	1.378 (4)	C24—H26	0.980
C17—C18	1.382 (5)	C24—H27	0.980
C18—C19	1.368 (4)		

N1—S1—N2	122.65 (10)	C6—C5—H3	119.615
N1—S1—C9	114.85 (10)	C1—C6—H4	120.640
N1—S1—C15	103.35 (11)	C5—C6—H4	120.642
N2—S1—C9	104.95 (11)	C3—C7—H5	109.464
N2—S1—C15	104.96 (10)	C3—C7—H6	109.466
C9—S1—C15	104.17 (10)	C3—C7—H7	109.465
S1—N1—C8	116.62 (17)	H5—C7—H6	109.487
S1—N2—C21	119.21 (14)	H5—C7—H7	109.474
S1—N2—C23	115.20 (17)	H6—C7—H7	109.470

C21—N2—C23	115.73 (19)	C9—C10—H8	121.216
C2—C1—C6	119.7 (3)	C11—C10—H8	121.202
C2—C1—C8	117.8 (3)	C10—C11—H9	119.576
C6—C1—C8	122.5 (2)	C12—C11—H9	119.586
C1—C2—C3	121.5 (3)	C11—C12—H10	119.725
C2—C3—C4	118.1 (3)	C13—C12—H10	119.724
C2—C3—C7	120.1 (3)	C12—C13—H11	119.844
C4—C3—C7	121.8 (3)	C14—C13—H11	119.836
C3—C4—C5	121.2 (3)	C9—C14—H12	121.085
C4—C5—C6	120.8 (3)	C13—C14—H12	121.089
C1—C6—C5	118.7 (3)	C15—C16—H13	121.107
O1—C8—N1	123.5 (2)	C17—C16—H13	121.105
O1—C8—C1	122.3 (2)	C16—C17—H14	119.482
N1—C8—C1	114.2 (3)	C18—C17—H14	119.470
S1—C9—C10	116.40 (18)	C17—C18—H15	120.093
S1—C9—C14	120.16 (16)	C19—C18—H15	120.090
C10—C9—C14	122.8 (2)	C18—C19—H16	119.526
C9—C10—C11	117.6 (3)	C20—C19—H16	119.523
C10—C11—C12	120.8 (3)	C15—C20—H17	121.092
C11—C12—C13	120.6 (3)	C19—C20—H17	121.089
C12—C13—C14	120.3 (3)	N2—C21—H18	109.466
C9—C14—C13	117.8 (2)	N2—C21—H19	109.463
S1—C15—C16	118.3 (2)	C22—C21—H18	109.463
S1—C15—C20	118.76 (17)	C22—C21—H19	109.464
C16—C15—C20	122.5 (3)	H18—C21—H19	108.058
C15—C16—C17	117.8 (3)	C21—C22—H20	109.479
C16—C17—C18	121.0 (3)	C21—C22—H21	109.469
C17—C18—C19	119.8 (3)	C21—C22—H22	109.477
C18—C19—C20	121.0 (3)	H20—C22—H21	109.466
C15—C20—C19	117.8 (3)	H20—C22—H22	109.469
N2—C21—C22	110.9 (3)	H21—C22—H22	109.467
N2—C23—C24	114.7 (3)	N2—C23—H23	108.586
F1—B1—F2	112.1 (4)	N2—C23—H24	108.588
F1—B1—F3	106.6 (3)	C24—C23—H23	108.594
F1—B1—F4	108.6 (4)	C24—C23—H24	108.588
F2—B1—F3	107.8 (3)	H23—C23—H24	107.553
F2—B1—F4	111.8 (3)	C23—C24—H25	109.471
F3—B1—F4	109.7 (4)	C23—C24—H26	109.469
C1—C2—H1	119.276	C23—C24—H27	109.466
C3—C2—H1	119.262	H25—C24—H26	109.476
C3—C4—H2	119.372	H25—C24—H27	109.474
C5—C4—H2	119.381	H26—C24—H27	109.471
C4—C5—H3	119.624		

N1—S1—N2—C21	−85.43 (16)	C2—C1—C8—O1	−3.4 (3)
N1—S1—N2—C23	58.94 (17)	C2—C1—C8—N1	175.71 (17)
N2—S1—N1—C8	62.03 (16)	C8—C1—C2—C3	−179.78 (16)
N1—S1—C9—C10	−9.7 (2)	C6—C1—C8—O1	175.96 (19)

N1—S1—C9—C14	178.86 (15)	C6—C1—C8—N1	−4.9 (3)
C9—S1—N1—C8	−67.35 (15)	C8—C1—C6—C5	179.28 (17)
N1—S1—C15—C16	−165.52 (13)	C1—C2—C3—C4	0.5 (3)
N1—S1—C15—C20	21.46 (16)	C1—C2—C3—C7	−178.65 (17)
C15—S1—N1—C8	179.88 (12)	C2—C3—C4—C5	−1.2 (4)
N2—S1—C9—C10	−147.38 (15)	C7—C3—C4—C5	177.9 (2)
N2—S1—C9—C14	41.21 (19)	C3—C4—C5—C6	0.7 (4)
C9—S1—N2—C21	48.02 (16)	C4—C5—C6—C1	0.6 (4)
C9—S1—N2—C23	−167.61 (12)	S1—C9—C10—C11	−173.55 (16)
N2—S1—C15—C16	−35.93 (16)	S1—C9—C14—C13	172.18 (16)
N2—S1—C15—C20	151.06 (14)	C10—C9—C14—C13	1.3 (4)
C15—S1—N2—C21	157.51 (13)	C14—C9—C10—C11	−2.4 (4)
C15—S1—N2—C23	−58.13 (15)	C9—C10—C11—C12	1.8 (4)
C9—S1—C15—C16	74.12 (15)	C10—C11—C12—C13	−0.2 (5)
C9—S1—C15—C20	−98.89 (15)	C11—C12—C13—C14	−0.9 (5)
C15—S1—C9—C10	102.56 (16)	C12—C13—C14—C9	0.3 (4)
C15—S1—C9—C14	−68.85 (18)	S1—C15—C16—C17	−174.46 (13)
S1—N1—C8—O1	−2.3 (3)	S1—C15—C20—C19	174.92 (14)
S1—N1—C8—C1	178.56 (11)	C16—C15—C20—C19	2.2 (4)
S1—N2—C21—C22	−148.33 (13)	C20—C15—C16—C17	−1.7 (3)
S1—N2—C23—C24	−85.0 (3)	C15—C16—C17—C18	−0.3 (4)
C21—N2—C23—C24	60.7 (3)	C16—C17—C18—C19	1.7 (4)
C23—N2—C21—C22	67.5 (3)	C17—C18—C19—C20	−1.2 (4)
C2—C1—C6—C5	−1.4 (3)	C18—C19—C20—C15	−0.7 (4)
C6—C1—C2—C3	0.8 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H6···F3^{i}	0.98	2.50	3.446 (4)	163
C10—H8···F4	0.95	2.48	3.202 (5)	133
C14—H12···F3^{ii}	0.95	2.51	3.433 (3)	165
C16—H13···F2^{ii}	0.95	2.61	3.367 (4)	137
C16—H13···F3^{ii}	0.95	2.55	3.450 (4)	158
C18—H15···F1^{iii}	0.95	2.33	3.200 (5)	150

Symmetry codes: (i) x, $-y-1/2$, $z-1/2$; (ii) x, $-y+1/2$, $z-1/2$; (iii) $-x+1$, $y+1/2$, $-z+3/2$.