



# Synthesis and crystal structures of two 1,3-di(alkyloxy)-2-(methylsulfanyl)imidazolium tetrafluoroborates

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Two salts were prepared by methylation of the respective imidazoline-2-thione at the sulfur atom, using Meerwein's salt (trimethyloxonium tetrafluoroborate) in CH<sub>2</sub>Cl<sub>2</sub>. 1,3-Dimethoxy-2-(methylsulfanyl)imidazolium tetrafluoroborate (**1**), C<sub>6</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub>S<sup>+</sup>·BF<sub>4</sub><sup>-</sup>, displays a *syn* conformation of its two methoxy groups relative to each other whereas the two benzyloxy groups present in 1,3-dibenzyloxy-2-(methylsulfanyl)imidazolium tetrafluoroborate (**2**), C<sub>18</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub>S<sup>+</sup>·BF<sub>4</sub><sup>-</sup>, adopt an *anti* conformation. In the molecules of **1** and **2**, the methylsulfanyl group is rotated out of the plane of the respective heterocyclic ring. In both crystal structures, intermolecular interactions are dominated by C—H···F—B contacts, leading to three-dimensional networks. The tetrafluoridoborate counter-ion of **2** is disordered over three orientations (occupancy ratio 0.42:0.34:0.24), which are related by rotation about one of the B—F bonds.

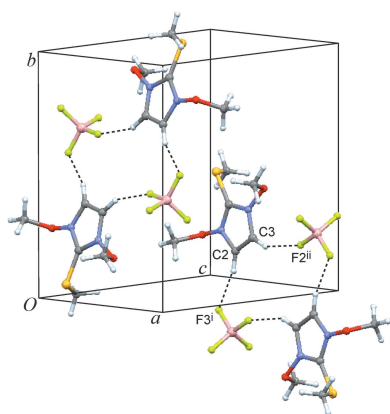
## 1. Chemical context

2-(Methylthio)imidazolium salts have attracted great interest because of their reactive properties. Compounds belonging to this class can be converted into important derivatives with useful biological activity, *i.e.* as anti-filarial agents (Link *et al.*, 1990). Furthermore, they have been used as precursors for the synthesis of remote *N*-heterocyclic carbene complexes (*r*NHC) (Patel *et al.*, 2018), as tunable alkylating reagents (Guterman *et al.*, 2018) or as coupling reagents for the formation of bis(2-imidazolyl)methyl salts (Kuhn *et al.*, 1993; Fürstner *et al.*, 2008).

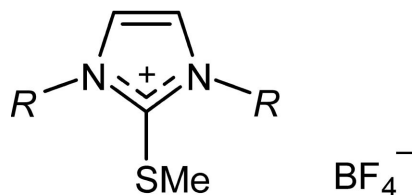
The S-methylation of thiones, typically with methyl iodide or Meerwein's salt (trimethyloxonium tetrafluoroborate), is straightforward. The title compounds **1** and **2** were prepared by methylation of 1,3-dimethoxyimidazoline-2-thione (Laus *et al.*, 2013) and 1,3-di(benzyloxy)imidazoline-2-thione (Laus *et al.*, 2016), respectively, using Meerwein's salt in CH<sub>2</sub>Cl<sub>2</sub>. An analogous procedure was applied by Williams *et al.* (1994) for the synthesis of the classic 1,3-dimethyl-2-(methylsulfanyl)imidazolium iodide.

## 2. Structural commentary

In the organic cation of **1**, the two methoxy groups adopt a *syn* conformation relative to each other, and the methylsulfanyl group is *anti* to each of the methoxy groups (Fig. 1). In contrast, the structurally related molecule of 1,3-dimethoxy-

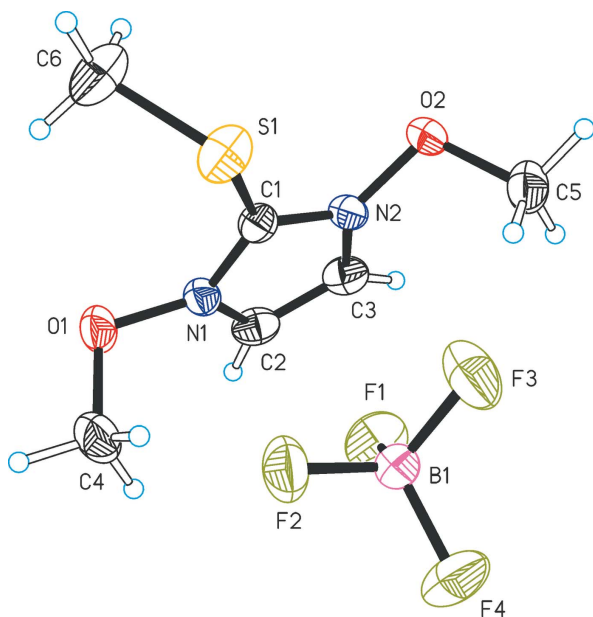


imidazoline-2-thione displays an *anti* conformation of its methoxy groups (Laus *et al.*, 2013). The two N–OMe fragments of **1** form dihedral angles with the mean plane of the imidazole ring of  $82.3(2)^\circ$  (for the ring involving O1 and C4) and of  $76.8(1)^\circ$  (for the ring involving O2 and C5). The methylsulfanyl group (S1–C6) is rotated out of the heterocyclic plane and forms a dihedral angle of  $62.5(1)^\circ$  with the mean plane of the heterocycle defined by atoms N1, C1, N2, C2, and C3.

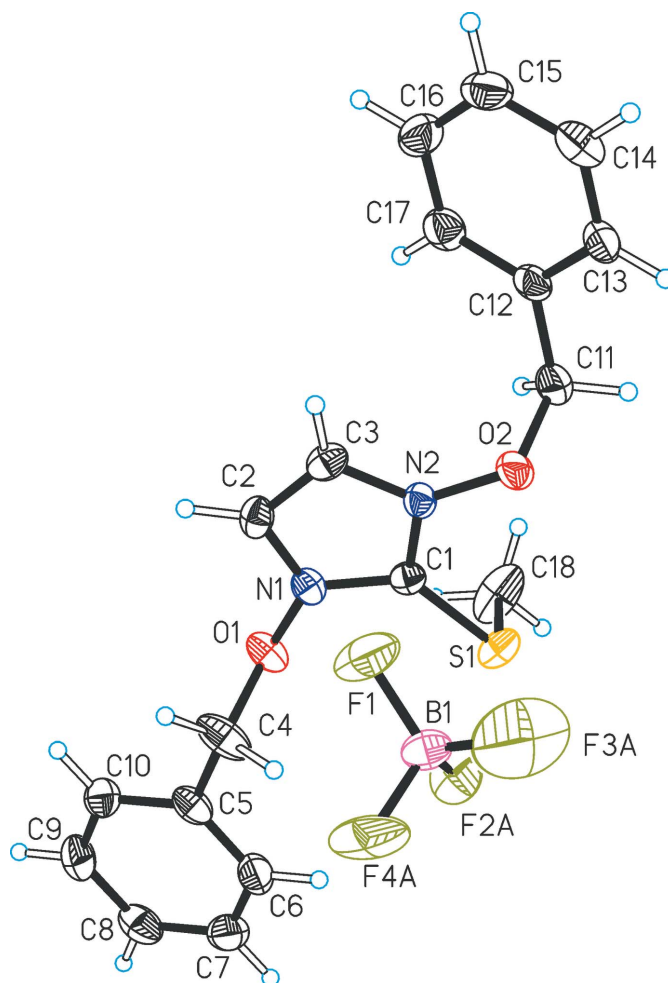


- 1**  $R = \text{OMe}$   
**2**  $R = \text{OBn}$

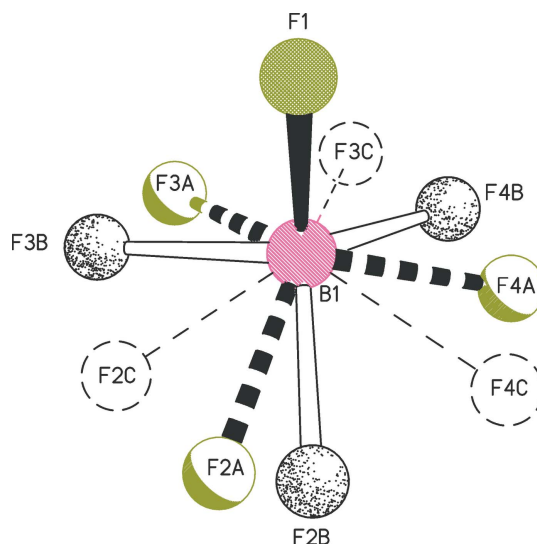
Similar to **1**, the methylsulfanyl group (S1–C18) of **2** is rotated out of the plane of the heterocycle and forms a dihedral angle of  $78.6(1)^\circ$  with the mean plane defined by the imidazole ring atoms (N1, C1, N2, C2, C3). The arrangement of the two benzyloxy moieties in the cation of **2** relative to each other is *anti* (Fig. 2). They adopt distinct conformations, which is illustrated by the different values of the torsion angles  $\text{N1–O1–C4–C5} = -174.2(2)^\circ$  and  $\text{N2–O2–C11–C12} = 95.5(2)^\circ$ . The two benzene ring planes are inclined by  $17.34(9)^\circ$  for C5–C10 and by  $30.6(1)^\circ$  for C12–C17 relative to the plane of the central heterocycle. The tetrafluoridoborate counter-ion of **2** is disordered over three orientations (occu-



**Figure 1**  
 The ion pair structure of methylsulfanyl salt **1**, showing displacement ellipsoids drawn at the 50% probability level and hydrogen atoms drawn as spheres of arbitrary size.



**Figure 2**  
 The ion pair structure of methylsulfanyl salt **2**, showing displacement ellipsoids drawn at the 50% probability level and hydrogen atoms drawn as spheres of arbitrary size. Only one of the three different orientations of the disordered  $\text{BF}_4^-$  anion is shown.



**Figure 3**  
 Disorder of the tetrafluoridoborate anion in the structure of **2**. The disorder components *A* (F2A, F3A, F4A), *B* (F2B, F3B, F4B) and *C* (F2C, F3C, F4C) are related by a rotation about the B1–F1 bond.

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2···F3 <sup>i</sup>	0.95	2.26	3.137 (3)	154
C2—H2···F2 <sup>i</sup>	0.95	2.51	3.361 (3)	150
C3—H3···F2 <sup>ii</sup>	0.95	2.33	3.207 (3)	153
C4—H4B···F3 <sup>iii</sup>	0.98	2.61	3.408 (3)	139
C4—H4B···F4 <sup>iii</sup>	0.98	2.52	3.487 (3)	168
C4—H4C···F2	0.98	2.46	3.418 (3)	167
C5—H5A···F3	0.98	2.54	3.519 (3)	177

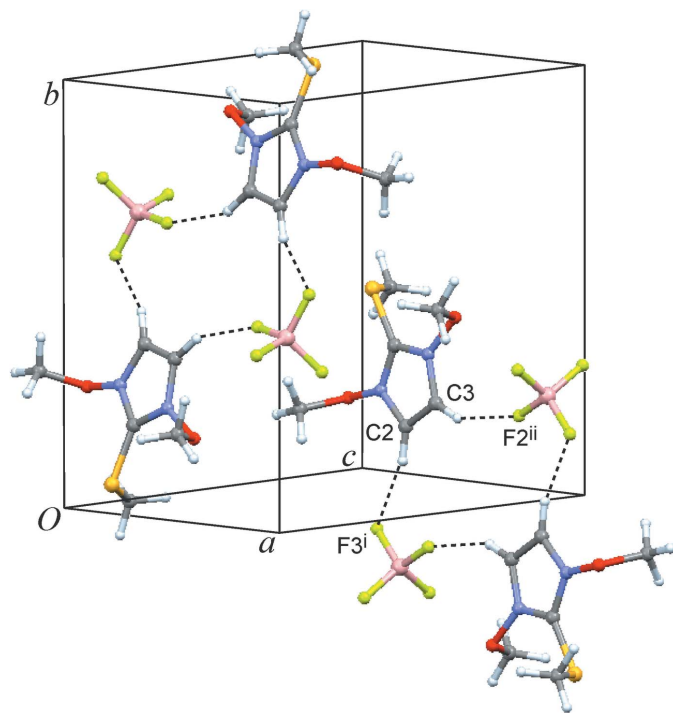
Symmetry codes: (i)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (iii)  $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ .

pancy ratio 0.42:0.34:0.24), which are related by a rotation about the B1—F1 bond (Fig. 3).

The heterocycle C—S bond lengths [1.722 (2) and 1.721 (3) Å for **1** and **2**, respectively] determined in this study are in good agreement with the mean value (1.735 Å) calculated from 82 pertinent C—S distances compiled in the Cambridge Structural Database (selection criterion  $R_1 < 0.10$ ; Groom *et al.*, 2016).

### 3. Supramolecular features

Both structures display multiple C—H···F—B contacts which cross-link the ion pairs and result in three-dimensional networks (Tables 1 and 2). In the crystal structure of **1**, the two most important of these interactions, C2—H2···F3( $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ) and C3—H3···F2( $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ), involve the two imidazole CH groups and yield a substructure with an



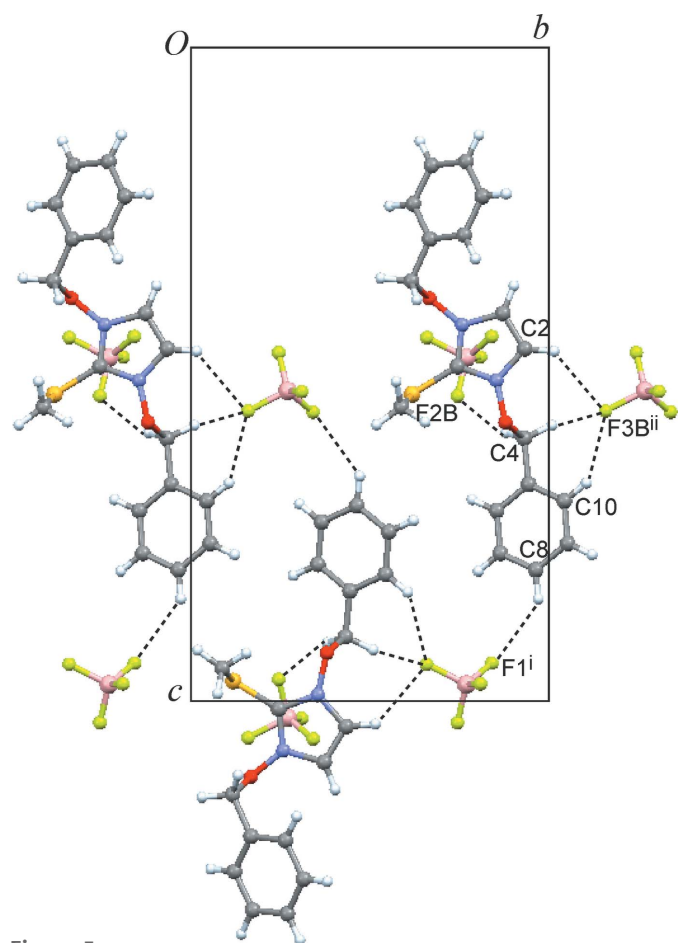
**Figure 4**  
Crystal packing of compound **1**. Dashed lines represent the shortest intermolecular C—H···F interactions. [Symmetry codes: (i)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ].

**Table 2**  
Hydrogen-bond geometry (Å, °) for **2**.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2···F2A <sup>i</sup>	0.95	2.28	3.200 (13)	162
C2—H2···F3B <sup>i</sup>	0.95	2.55	3.302 (14)	136
C2—H2···F2C <sup>i</sup>	0.95	2.07	2.936 (10)	150
C4—H4B···F2B	0.99	2.52	3.472 (17)	162
C4—H4A···F3B <sup>i</sup>	0.99	2.50	3.183 (13)	126
C4—H4A···F2C <sup>i</sup>	0.99	2.56	3.39 (3)	141
C4—H4B···F4C	0.99	2.61	3.522 (19)	153
C8—H8···F1 <sup>ii</sup>	0.95	2.54	3.317 (4)	139
C10—H10···F3B <sup>i</sup>	0.95	2.46	3.282 (12)	145
C11—H11A···F3A <sup>iii</sup>	0.99	2.27	3.247 (13)	167
C11—H11A···F3C <sup>iii</sup>	0.99	2.40	3.279 (15)	148
C18—H18C···F3A <sup>iii</sup>	0.98	2.62	3.409 (14)	138

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

$R_4^4(14)$  motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995) (Fig. 4). Moreover, the two methoxy groups are involved in this type of hydrogen bonding, albeit with weaker strength as can be seen in the longer H···F contacts (Table 1). In the di(benzyloxy) salt **2**, each of the three disorder components of the anion gives rise to a specific set of C—H···F—B contacts. Fig. 5 shows the most significant interactions for one of the  $\text{BF}_4^-$



**Figure 5**  
Crystal packing of compound **2**, viewed along the *a* axis. Dashed lines represent the shortest intermolecular C—H···F interactions involving the disorder component *B* of the tetrafluoroborate anion. [Symmetry codes: (i)  $-x + 1, y, z + \frac{1}{2}$ ; (ii)  $-x + 1, y + \frac{1}{2}, -z + 1$ ].

**Table 3**  
Experimental details.

	1	2
Crystal data		
Chemical formula	C <sub>6</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub> S <sup>+</sup> ·BF <sub>4</sub> <sup>-</sup>	C <sub>18</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub> S <sup>+</sup> ·BF <sub>4</sub> <sup>-</sup>
<i>M<sub>r</sub></i>	262.04	414.22
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>	Orthorhombic, <i>P</i> c2 <sub>1</sub> / <i>b</i>
Temperature (K)	173	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.1049 (7), 11.6979 (10), 12.0810 (12)	7.9117 (3), 11.4760 (4), 20.9659 (7)
$\alpha$ , $\beta$ , $\gamma$ (°)	90, 90.069 (9), 90	90, 90, 90
<i>V</i> (Å <sup>3</sup> )	1145.40 (18)	1903.59 (12)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
$\mu$ (mm <sup>-1</sup> )	0.32	0.22
Crystal size (mm)	0.20 × 0.14 × 0.12	0.44 × 0.36 × 0.12
Data collection		
Diffractometer	Rigaku Oxford Diffraction Xcalibur, Ruby, Gemini ultra	Rigaku Oxford Diffraction Xcalibur, Ruby, Gemini ultra
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku OD, 2015)	Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku OD, 2015)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.973, 1	0.936, 1
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	8186, 2175, 1640	11654, 3555, 3293
<i>R</i> <sub>int</sub>	0.041	0.029
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.610	0.610
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.037, 0.088, 1.04	0.030, 0.067, 1.06
No. of reflections	2175	3555
No. of parameters	148	311
No. of restraints	0	368
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.25, -0.26	0.18, -0.23
Absolute structure	–	Flack <i>x</i> determined using 1454 quotients [( <i>I</i> <sup>+</sup> ) - ( <i>I</i> <sup>-</sup> )] / [( <i>I</i> <sup>+</sup> ) + ( <i>I</i> <sup>-</sup> )] (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	–	0.02 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SIR2002* (Burla *et al.*, 2003), *SHELXL2014/6* (Sheldrick, 2015), *XP/SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

components, which also involves one heterocyclic hydrogen (H2) as well as both methylene (H4A, H4B; H11A) and two aromatic hydrogen atoms (H8, H10) of the cation. In contrast to **1**, the methylsulfanyl group (H18C) is also involved in hydrogen-bonding interactions.

#### 4. Database survey

In addition to the classic 1,3-dimethylimidazolium-2-methylsulfanylimidazolium iodide (Williams *et al.*, 1994), the Cambridge Structural Database (Version 5.41 November 2019; Groom *et al.*, 2016) comprises a number of more unusual representatives such as very bulky 1,3-diaryl-2-phenylthioimidazolium (Inés *et al.*, 2010) and 1,3-diaryl-2-methylsulfanylimidazolium salts (Liu *et al.*, 2017). These compounds are suitable precursors for the generation of exotic *N*-heterocyclic carbene–chalcogen cations.

Noteworthy is also the structure of a stabilized imidazoline-2-thione methylide (Arduengo & Burgess, 1976). The attachment of a fluorine-containing group to a given molecule may enhance certain properties and therefore widen the range of potential applications. For example, salts bearing S–CF<sub>3</sub> groups (Mizuta *et al.*, 2016) have been found to be effective electrophilic phase-transfer catalysts. Additionally, the intro-

duction of perfluoroalkylthio groups (Hummel *et al.*, 2017) resulted in improved surfactant properties.

#### 5. Synthesis and crystallization

**1,3-Dimethoxy-2-methylsulfanylimidazolium tetrafluoroborate (1):** Trimethyloxonium tetrafluoroborate (0.51 g, 3.44 mmol) was added to a solution of 1,3-dimethoxyimidazoline-2-thione (0.50 g, 3.12 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (20 ml). The mixture was stirred for 18 h at room temperature, then the solvent was evaporated. The residue was dissolved in EtOH (3 ml) and cooled at 277 K, forming colourless single crystals. The crystalline product was filtered, washed with Et<sub>2</sub>O (2 × 5 ml) and dried. Yield: 0.53 g, m.p. 363 K. <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>): δ 2.72 (*s*, 3H), 4.25 (*s*, 6H), 8.43 (*s*, 2H) ppm <sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>): δ 16.3, 68.9 (2C), 118.0 (2C), 135.7 ppm IR (neat): ν 3153 (*m*), 3134 (*m*), 1552 (*m*), 1445 (*m*), 1287 (*w*), 1043 (*vs*), 1018 (*vs*), 937 (*s*), 754 (*s*), 734 (*s*), 689 (*m*), 672 (*m*), 619 (*m*), 520 (*s*) cm<sup>-1</sup>.

**1,3-Di(benzyloxy)-2-methylsulfanylimidazolium tetrafluoroborate (2):** Trimethyloxonium tetrafluoroborate (0.26 g, 1.7 mmol) was added to a solution of 1,3-di(benzyloxy)imidazoline-2-thione (0.51 g, 1.6 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (8 ml) in a Teflon test tube under argon. The mixture was

stirred for 3 d at room temperature, then the solvent was evaporated. The residue was dissolved in MeOH (15 ml), precipitated with Et<sub>2</sub>O (15 ml), filtered, washed with Et<sub>2</sub>O and dried to yield a colourless powder. Single crystals were obtained by slow evaporation from an MeOH solution: Yield 0.42 g (62%), m.p. 407 K. <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>): δ 2.54 (*s*, 3H), 5.45 (*s*, 4H), 7.49 (*s*, 10H), 8.36 (*s*, 2H) ppm <sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>): δ 16.4, 83.1 (2C), 118.9 (2C), 128.9 (4C), 130.2 (2C), 130.4 (4C), 131.8 (2C), 136.8 ppm IR (neat): ν 3167 (*w*), 3137 (*w*), 1550 (*w*), 1492 (*w*), 1457 (*w*), 1384 (*w*), 1354 (*w*), 1214 (*w*), 1057 (*vs*), 1039 (*vs*), 907 (*m*), 873 (*m*), 844 (*m*), 773 (*s*), 739 (*s*), 699 (*s*), 671 (*s*), 575 (*m*), 499 (*m*) cm<sup>-1</sup>.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All hydrogen atoms were identified in difference maps. Methyl H atoms were idealized and included as rigid groups allowed to rotate but not tip (C–H = 0.98 Å), and their *U*<sub>iso</sub> parameters were set to 1.5 *U*<sub>eq</sub>(C) of the parent carbon atom. H atoms bonded to secondary carbon atoms (C–H = 0.99 Å), and H atoms bonded to C atoms in aromatic rings (C–H = 0.95 Å) were positioned geometrically and refined with *U*<sub>iso</sub> set to 1.2 *U*<sub>eq</sub>(C) of the parent carbon atom.

The structure of **2** displays disorder of the tetrafluoroborate ion involving three distinct components. Therefore, distance restraints were applied for all chemically equivalent B–F and F···F distances and restraints on displacement parameters of the F atoms affected by disorder were applied.

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## supporting information

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## Synthesis and crystal structures of two 1,3-di(alkyloxy)-2-(methylsulfanyl)imidazolium tetrafluoridoborates

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### Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL2014/6* (Sheldrick, 2015); molecular graphics: *XP/SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### 1,3-Dimethoxy-2-(methylsulfanyl)imidazolium tetrafluoridoborate (1)

#### Crystal data

$C_6H_{11}N_2O_2S^+ \cdot BF_4^-$   
 $M_r = 262.04$   
 Monoclinic,  $P2_1/n$   
 $a = 8.1049$  (7) Å  
 $b = 11.6979$  (10) Å  
 $c = 12.0810$  (12) Å  
 $\beta = 90.069$  (9)°  
 $V = 1145.40$  (18) Å<sup>3</sup>  
 $Z = 4$

$F(000) = 536$   
 $D_x = 1.520$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 1882 reflections  
 $\theta = 4.5\text{--}23.4^\circ$   
 $\mu = 0.32$  mm<sup>-1</sup>  
 $T = 173$  K  
 Block, colourless  
 $0.20 \times 0.14 \times 0.12$  mm

#### Data collection

Rigaku Oxford Diffraction Xcalibur, Ruby,  
 Gemini ultra  
 diffractometer  
 Radiation source: fine-focus sealed X-ray tube,  
 Enhance (Mo) X-ray Source  
 Graphite monochromator  
 Detector resolution: 10.3575 pixels mm<sup>-1</sup>  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (CrysAlisPro; Rigaku OD, 2015)

$T_{\min} = 0.973$ ,  $T_{\max} = 1$   
 8186 measured reflections  
 2175 independent reflections  
 1640 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$   
 $\theta_{\max} = 25.7^\circ$ ,  $\theta_{\min} = 3.4^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -14 \rightarrow 14$   
 $l = -11 \rightarrow 14$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.088$   
 $S = 1.04$

2175 reflections  
 148 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

$$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 0.4296P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.41330 (7)	0.47008 (5)	0.72979 (5)	0.03744 (19)
F1	0.08382 (16)	0.25059 (12)	0.80034 (13)	0.0477 (4)
F2	-0.01740 (16)	0.36253 (12)	0.66193 (10)	0.0439 (4)
F3	-0.0285 (2)	0.42160 (11)	0.83926 (11)	0.0516 (4)
F4	-0.18980 (16)	0.27590 (12)	0.78296 (13)	0.0514 (4)
O1	0.46146 (18)	0.22793 (13)	0.61505 (12)	0.0344 (4)
O2	0.45275 (18)	0.38275 (13)	0.97279 (12)	0.0340 (4)
N2	0.4484 (2)	0.30437 (14)	0.88842 (14)	0.0255 (4)
N1	0.4543 (2)	0.23500 (14)	0.72783 (14)	0.0251 (4)
C1	0.4420 (2)	0.33444 (17)	0.78163 (17)	0.0246 (5)
C2	0.4692 (2)	0.14498 (18)	0.79882 (19)	0.0304 (5)
H2	0.4810	0.0667	0.7796	0.036*
C3	0.4638 (2)	0.18919 (18)	0.90157 (19)	0.0301 (5)
H3	0.4696	0.1484	0.9695	0.036*
C5	0.2956 (3)	0.3860 (2)	1.0302 (2)	0.0389 (6)
H5A	0.2067	0.3988	0.9766	0.058*
H5B	0.2965	0.4482	1.0845	0.058*
H5C	0.2775	0.3131	1.0683	0.058*
C6	0.6002 (3)	0.4910 (2)	0.6533 (2)	0.0477 (7)
H6A	0.6951	0.4823	0.7029	0.072*
H6B	0.6007	0.5680	0.6213	0.072*
H6C	0.6069	0.4343	0.5938	0.072*
B1	-0.0377 (3)	0.3266 (2)	0.7711 (2)	0.0276 (6)
C4	0.3017 (3)	0.1968 (2)	0.5703 (2)	0.0471 (7)
H4A	0.2681	0.1226	0.6004	0.071*
H4B	0.3088	0.1917	0.4895	0.071*
H4C	0.2203	0.2549	0.5908	0.071*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0346 (3)	0.0294 (3)	0.0484 (4)	0.0073 (2)	0.0086 (3)	0.0077 (3)
F1	0.0337 (8)	0.0490 (9)	0.0605 (10)	0.0094 (6)	-0.0015 (7)	0.0051 (7)
F2	0.0500 (8)	0.0562 (9)	0.0254 (7)	0.0007 (7)	0.0062 (6)	0.0000 (6)

F3	0.0889 (12)	0.0336 (8)	0.0323 (8)	-0.0033 (7)	0.0035 (7)	-0.0043 (6)
F4	0.0278 (7)	0.0643 (10)	0.0621 (10)	-0.0099 (7)	-0.0001 (7)	0.0120 (8)
O1	0.0272 (8)	0.0512 (10)	0.0247 (9)	-0.0011 (7)	0.0056 (6)	-0.0087 (7)
O2	0.0307 (8)	0.0409 (9)	0.0305 (9)	-0.0101 (7)	0.0022 (7)	-0.0140 (7)
N2	0.0237 (9)	0.0262 (9)	0.0266 (10)	-0.0035 (7)	-0.0003 (7)	-0.0059 (8)
N1	0.0219 (9)	0.0292 (10)	0.0242 (10)	-0.0009 (7)	0.0008 (7)	-0.0048 (8)
C1	0.0183 (10)	0.0277 (11)	0.0276 (12)	0.0007 (9)	0.0019 (9)	-0.0019 (10)
C2	0.0243 (11)	0.0254 (11)	0.0415 (14)	-0.0001 (9)	-0.0022 (10)	0.0010 (10)
C3	0.0277 (11)	0.0289 (12)	0.0337 (14)	-0.0020 (9)	-0.0052 (10)	0.0052 (10)
C5	0.0343 (13)	0.0493 (15)	0.0331 (13)	0.0004 (11)	0.0069 (10)	-0.0069 (11)
C6	0.0413 (15)	0.0406 (14)	0.0613 (18)	0.0012 (12)	0.0150 (13)	0.0150 (13)
B1	0.0253 (13)	0.0294 (13)	0.0282 (14)	-0.0015 (11)	0.0014 (10)	-0.0017 (11)
C4	0.0339 (13)	0.0779 (19)	0.0294 (14)	-0.0056 (13)	-0.0041 (11)	-0.0124 (13)

*Geometric parameters (Å, °)*

S1—C1	1.722 (2)	N1—C2	1.363 (3)
S1—C6	1.792 (2)	C2—C3	1.346 (3)
F1—B1	1.373 (3)	C2—H2	0.9500
F2—B1	1.394 (3)	C3—H3	0.9500
F3—B1	1.385 (3)	C5—H5A	0.9800
F4—B1	1.376 (3)	C5—H5B	0.9800
O1—N1	1.366 (2)	C5—H5C	0.9800
O1—C4	1.449 (3)	C6—H6A	0.9800
O2—N2	1.372 (2)	C6—H6B	0.9800
O2—C5	1.451 (3)	C6—H6C	0.9800
N2—C1	1.338 (3)	C4—H4A	0.9800
N2—C3	1.362 (3)	C4—H4B	0.9800
N1—C1	1.336 (3)	C4—H4C	0.9800
C1—S1—C6	101.52 (10)	O2—C5—H5C	109.5
N1—O1—C4	110.37 (15)	H5A—C5—H5C	109.5
N2—O2—C5	110.52 (15)	H5B—C5—H5C	109.5
C1—N2—C3	112.08 (17)	S1—C6—H6A	109.5
C1—N2—O2	122.80 (17)	S1—C6—H6B	109.5
C3—N2—O2	124.90 (17)	H6A—C6—H6B	109.5
C1—N1—C2	111.90 (18)	S1—C6—H6C	109.5
C1—N1—O1	122.75 (17)	H6A—C6—H6C	109.5
C2—N1—O1	125.22 (17)	H6B—C6—H6C	109.5
N1—C1—N2	103.73 (17)	F1—B1—F4	109.66 (19)
N1—C1—S1	129.46 (17)	F1—B1—F3	109.20 (19)
N2—C1—S1	126.73 (16)	F4—B1—F3	109.36 (18)
C3—C2—N1	106.29 (19)	F1—B1—F2	110.68 (18)
C3—C2—H2	126.9	F4—B1—F2	109.58 (19)
N1—C2—H2	126.9	F3—B1—F2	108.32 (18)
C2—C3—N2	106.00 (19)	O1—C4—H4A	109.5
C2—C3—H3	127.0	O1—C4—H4B	109.5
N2—C3—H3	127.0	H4A—C4—H4B	109.5



O2—C5—H5A	109.5	O1—C4—H4C	109.5
O2—C5—H5B	109.5	H4A—C4—H4C	109.5
H5A—C5—H5B	109.5	H4B—C4—H4C	109.5

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ F3 <sup>i</sup>	0.95	2.26	3.137 (3)	154
C2—H2 $\cdots$ F2 <sup>i</sup>	0.95	2.51	3.361 (3)	150
C3—H3 $\cdots$ F2 <sup>ii</sup>	0.95	2.33	3.207 (3)	153
C4—H4B $\cdots$ F3 <sup>iii</sup>	0.98	2.61	3.408 (3)	139
C4—H4B $\cdots$ F4 <sup>iii</sup>	0.98	2.52	3.487 (3)	168
C4—H4C $\cdots$ F2	0.98	2.46	3.418 (3)	167
C5—H5A $\cdots$ F3	0.98	2.54	3.519 (3)	177

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

1,3-Dibenzyloxy-2-(methylsulfanyl)imidazolium tetrafluoridoborate (2)

Crystal data

$C_{18}H_{19}N_2O_2S^+ \cdot BF_4^-$

$M_r = 414.22$

Orthorhombic,  $Pc2_1b$

Hall symbol: P -2bc -2c

$a = 7.9117$  (3)  $\text{\AA}$

$b = 11.4760$  (4)  $\text{\AA}$

$c = 20.9659$  (7)  $\text{\AA}$

$V = 1903.59$  (12)  $\text{\AA}^3$

$Z = 4$

$F(000) = 856$

$D_x = 1.445$  Mg  $\text{m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$   $\text{\AA}$

Cell parameters from 6176 reflections

$\theta = 3.1\text{--}28.6^\circ$

$\mu = 0.22$   $\text{mm}^{-1}$

$T = 173$  K

Plate, colourless

$0.44 \times 0.36 \times 0.12$  mm

Data collection

Rigaku Oxford Diffraction Xcalibur, Ruby,  
Gemini ultra  
diffractometer

Graphite monochromator

Detector resolution: 10.3575 pixels  $\text{mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan  
(CrysAlisPro; Rigaku OD, 2015)

$T_{\min} = 0.936, T_{\max} = 1$

11654 measured reflections

3555 independent reflections

3293 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 25.7^\circ, \theta_{\min} = 3.2^\circ$

$h = -9 \rightarrow 8$

$k = -13 \rightarrow 13$

$l = -19 \rightarrow 25$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.067$

$S = 1.06$

3555 reflections

311 parameters

368 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

$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 0.3041P]$

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

$(\Delta/\sigma)_{\max} = 0.007$

$\Delta\rho_{\max} = 0.18$  e  $\text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.22$  e  $\text{\AA}^{-3}$

Absolute structure: Flack  $x$  determined using  
1454 quotients  $[(F^-)-(F)]/[(F^+)+(F)]$  (Parsons *et al.*, 2013).

Absolute structure parameter: 0.02 (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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
B1	0.7773 (4)	0.7700 (3)	0.47458 (15)	0.0309 (7)	
F1	0.6678 (2)	0.84120 (18)	0.44219 (10)	0.0588 (6)	
F2B	0.719 (2)	0.7454 (15)	0.5332 (6)	0.071 (6)	0.341 (5)
F3B	0.781 (3)	0.6596 (8)	0.4439 (7)	0.072 (5)	0.341 (5)
F4B	0.9356 (13)	0.8091 (14)	0.4735 (12)	0.083 (9)	0.341 (5)
F2C	0.7136 (18)	0.6688 (14)	0.4845 (18)	0.093 (7)	0.238 (4)
F3C	0.9288 (16)	0.7723 (19)	0.4449 (8)	0.060 (6)	0.238 (4)
F4C	0.803 (3)	0.834 (2)	0.5316 (6)	0.089 (6)	0.238 (4)
F2A	0.6947 (13)	0.7094 (11)	0.5212 (5)	0.044 (3)	0.421 (4)
F3A	0.849 (2)	0.6901 (17)	0.4354 (6)	0.126 (8)	0.421 (4)
F4A	0.9031 (14)	0.8315 (12)	0.5042 (8)	0.076 (5)	0.421 (4)
S1	0.33131 (8)	0.61824 (6)	0.53046 (3)	0.02961 (17)	
O2	0.3430 (2)	0.66702 (16)	0.38403 (8)	0.0283 (4)	
O1	0.2637 (2)	0.87919 (17)	0.57345 (8)	0.0273 (4)	
N1	0.2835 (2)	0.85434 (19)	0.50947 (9)	0.0223 (5)	
N2	0.3093 (2)	0.75797 (18)	0.42440 (10)	0.0214 (5)	
C1	0.3058 (3)	0.7453 (2)	0.48800 (12)	0.0208 (5)	
C3	0.2924 (3)	0.8725 (2)	0.40683 (12)	0.0256 (6)	
H3	0.2937	0.9028	0.3647	0.031*	
C12	0.1490 (3)	0.6677 (2)	0.29313 (12)	0.0261 (6)	
C9	0.2992 (3)	1.0534 (3)	0.75895 (14)	0.0350 (7)	
H9	0.2491	1.1218	0.7762	0.042*	
C10	0.3228 (3)	1.0439 (3)	0.69382 (13)	0.0304 (6)	
H10	0.2893	1.1057	0.6665	0.036*	
C5	0.3952 (3)	0.9444 (2)	0.66841 (12)	0.0280 (6)	
C6	0.4421 (4)	0.8550 (3)	0.70894 (13)	0.0342 (7)	
H6	0.4907	0.7860	0.6919	0.041*	
C11	0.1862 (3)	0.6160 (3)	0.35716 (12)	0.0314 (6)	
H11A	0.0904	0.6312	0.3864	0.038*	
H11B	0.1995	0.5305	0.3530	0.038*	
C15	0.0978 (4)	0.7695 (3)	0.17451 (14)	0.0389 (7)	
H15	0.0811	0.8047	0.1340	0.047*	
C17	0.0445 (3)	0.7640 (3)	0.28694 (13)	0.0331 (6)	
H17	-0.0103	0.7953	0.3234	0.040*	
C2	0.2736 (3)	0.9333 (2)	0.46104 (12)	0.0252 (6)	
H2	0.2567	1.0150	0.4649	0.030*	
C7	0.4189 (4)	0.8652 (3)	0.77389 (14)	0.0392 (7)	
H7	0.4521	0.8034	0.8013	0.047*	
C8	0.3482 (4)	0.9641 (3)	0.79913 (14)	0.0369 (7)	

H8	0.3329	0.9712	0.8439	0.044*
C4	0.4199 (4)	0.9319 (3)	0.59824 (13)	0.0405 (8)
H4A	0.4396	1.0090	0.5783	0.049*
H4B	0.5183	0.8812	0.5891	0.049*
C13	0.2265 (3)	0.6217 (3)	0.23927 (12)	0.0318 (6)
H13	0.2976	0.5554	0.2429	0.038*
C18	0.1150 (4)	0.5878 (3)	0.55032 (17)	0.0498 (9)
H18A	0.0666	0.6545	0.5731	0.075*
H18B	0.1098	0.5185	0.5775	0.075*
H18C	0.0506	0.5738	0.5111	0.075*
C14	0.2001 (4)	0.6726 (3)	0.18030 (14)	0.0396 (7)
H14	0.2527	0.6406	0.1435	0.047*
C16	0.0199 (4)	0.8148 (3)	0.22780 (14)	0.0389 (7)
H16	-0.0511	0.8812	0.2239	0.047*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
B1	0.0229 (16)	0.040 (2)	0.0298 (17)	0.0004 (14)	-0.0001 (12)	0.0065 (16)
F1	0.0409 (11)	0.0542 (13)	0.0813 (14)	-0.0050 (9)	-0.0231 (9)	0.0296 (11)
F2B	0.102 (13)	0.081 (13)	0.029 (4)	0.002 (9)	0.017 (5)	-0.004 (6)
F3B	0.136 (16)	0.027 (4)	0.052 (7)	-0.007 (7)	-0.004 (8)	-0.014 (4)
F4B	0.025 (4)	0.051 (9)	0.17 (3)	0.002 (4)	0.011 (10)	0.043 (14)
F2C	0.066 (9)	0.037 (10)	0.17 (2)	-0.010 (7)	-0.002 (14)	0.053 (14)
F3C	0.031 (7)	0.087 (16)	0.061 (8)	0.015 (7)	0.020 (5)	-0.001 (8)
F4C	0.092 (12)	0.138 (17)	0.037 (6)	0.040 (11)	-0.013 (7)	-0.024 (8)
F2A	0.039 (3)	0.038 (6)	0.055 (7)	-0.012 (4)	0.007 (4)	0.014 (5)
F3A	0.101 (10)	0.21 (2)	0.071 (6)	0.089 (12)	0.018 (7)	-0.037 (11)
F4A	0.044 (7)	0.073 (8)	0.110 (11)	-0.038 (7)	-0.047 (7)	0.047 (7)
S1	0.0245 (3)	0.0282 (3)	0.0362 (4)	0.0029 (3)	0.0005 (2)	0.0108 (3)
O2	0.0270 (9)	0.0310 (10)	0.0269 (9)	0.0062 (8)	-0.0021 (7)	-0.0098 (8)
O1	0.0244 (9)	0.0357 (11)	0.0217 (9)	-0.0087 (8)	0.0059 (6)	-0.0073 (8)
N1	0.0218 (10)	0.0238 (12)	0.0211 (11)	-0.0014 (9)	0.0033 (8)	-0.0032 (9)
N2	0.0207 (10)	0.0211 (12)	0.0225 (11)	0.0024 (9)	0.0010 (8)	-0.0032 (9)
C1	0.0180 (11)	0.0229 (14)	0.0214 (13)	-0.0012 (10)	0.0001 (9)	0.0016 (11)
C3	0.0226 (12)	0.0271 (14)	0.0271 (13)	-0.0004 (11)	0.0009 (9)	0.0071 (13)
C12	0.0228 (12)	0.0268 (14)	0.0285 (13)	-0.0044 (11)	-0.0056 (10)	-0.0050 (12)
C9	0.0378 (15)	0.0281 (16)	0.0390 (16)	0.0001 (12)	0.0049 (12)	-0.0099 (14)
C10	0.0317 (14)	0.0248 (15)	0.0345 (15)	-0.0033 (12)	-0.0019 (11)	0.0027 (13)
C5	0.0228 (13)	0.0330 (15)	0.0281 (14)	-0.0099 (11)	0.0013 (10)	-0.0051 (12)
C6	0.0286 (14)	0.0287 (16)	0.0454 (17)	0.0007 (12)	-0.0035 (11)	-0.0099 (14)
C11	0.0370 (14)	0.0239 (13)	0.0332 (14)	-0.0047 (13)	-0.0049 (10)	-0.0033 (15)
C15	0.0431 (17)	0.0391 (18)	0.0345 (16)	-0.0097 (14)	-0.0149 (13)	0.0054 (14)
C17	0.0259 (13)	0.0358 (17)	0.0376 (16)	0.0009 (12)	-0.0036 (11)	-0.0079 (14)
C2	0.0213 (13)	0.0197 (13)	0.0346 (15)	-0.0018 (10)	0.0032 (10)	0.0007 (12)
C7	0.0406 (17)	0.0327 (17)	0.0443 (17)	-0.0056 (13)	-0.0148 (12)	0.0075 (16)
C8	0.0434 (18)	0.0428 (18)	0.0244 (15)	-0.0114 (14)	-0.0016 (12)	-0.0032 (13)
C4	0.0281 (14)	0.061 (2)	0.0327 (15)	-0.0200 (14)	0.0055 (12)	-0.0142 (15)

C13	0.0338 (14)	0.0274 (14)	0.0341 (15)	0.0017 (13)	-0.0056 (10)	-0.0108 (15)
C18	0.0327 (16)	0.042 (2)	0.074 (2)	0.0042 (14)	0.0209 (15)	0.0267 (17)
C14	0.0437 (17)	0.0448 (18)	0.0302 (15)	-0.0041 (15)	-0.0035 (13)	-0.0108 (14)
C16	0.0351 (16)	0.0323 (17)	0.049 (2)	0.0020 (13)	-0.0142 (13)	0.0023 (14)

*Geometric parameters (Å, °)*

B1—F2C	1.283 (11)	C9—H9	0.9500
B1—F4B	1.330 (10)	C10—C5	1.384 (4)
B1—F2B	1.342 (11)	C10—H10	0.9500
B1—F3C	1.350 (11)	C5—C6	1.383 (4)
B1—F3A	1.355 (10)	C5—C4	1.491 (4)
B1—F2A	1.367 (8)	C6—C7	1.379 (4)
B1—F4A	1.369 (9)	C6—H6	0.9500
B1—F1	1.371 (4)	C11—H11A	0.9900
B1—F4C	1.414 (12)	C11—H11B	0.9900
B1—F3B	1.422 (9)	C15—C16	1.378 (4)
S1—C1	1.721 (3)	C15—C14	1.381 (5)
S1—C18	1.795 (3)	C15—H15	0.9500
O2—N2	1.370 (3)	C17—C16	1.384 (4)
O2—C11	1.483 (3)	C17—H17	0.9500
O1—N1	1.380 (3)	C2—H2	0.9500
O1—C4	1.471 (3)	C7—C8	1.372 (5)
N1—C1	1.341 (3)	C7—H7	0.9500
N1—C2	1.363 (3)	C8—H8	0.9500
N2—C1	1.342 (3)	C4—H4A	0.9900
N2—C3	1.372 (3)	C4—H4B	0.9900
C3—C2	1.342 (4)	C13—C14	1.383 (4)
C3—H3	0.9500	C13—H13	0.9500
C12—C17	1.386 (4)	C18—H18A	0.9800
C12—C13	1.389 (4)	C18—H18B	0.9800
C12—C11	1.497 (4)	C18—H18C	0.9800
C9—C8	1.382 (4)	C14—H14	0.9500
C9—C10	1.383 (4)	C16—H16	0.9500
F4B—B1—F2B	114.1 (10)	C7—C6—C5	120.6 (3)
F2C—B1—F3C	116.1 (11)	C7—C6—H6	119.7
F3A—B1—F2A	106.7 (8)	C5—C6—H6	119.7
F3A—B1—F4A	108.8 (8)	O2—C11—C12	110.4 (2)
F2A—B1—F4A	106.6 (7)	O2—C11—H11A	109.6
F2C—B1—F1	111.8 (7)	C12—C11—H11A	109.6
F4B—B1—F1	112.7 (7)	O2—C11—H11B	109.6
F2B—B1—F1	111.3 (8)	C12—C11—H11B	109.6
F3C—B1—F1	108.8 (8)	H11A—C11—H11B	108.1
F3A—B1—F1	111.5 (6)	C16—C15—C14	119.7 (3)
F2A—B1—F1	110.8 (5)	C16—C15—H15	120.2
F4A—B1—F1	112.2 (6)	C14—C15—H15	120.2
F2C—B1—F4C	112.7 (11)	C16—C17—C12	120.3 (3)

F3C—B1—F4C	104.6 (10)	C16—C17—H17	119.9
F1—B1—F4C	101.7 (6)	C12—C17—H17	119.9
F4B—B1—F3B	105.9 (8)	C3—C2—N1	106.2 (2)
F2B—B1—F3B	103.5 (8)	C3—C2—H2	126.9
F1—B1—F3B	108.6 (7)	N1—C2—H2	126.9
C1—S1—C18	99.97 (13)	C8—C7—C6	120.3 (3)
N2—O2—C11	111.87 (18)	C8—C7—H7	119.8
N1—O1—C4	109.43 (17)	C6—C7—H7	119.8
C1—N1—C2	112.2 (2)	C7—C8—C9	119.5 (3)
C1—N1—O1	122.3 (2)	C7—C8—H8	120.2
C2—N1—O1	125.5 (2)	C9—C8—H8	120.2
C1—N2—O2	122.4 (2)	O1—C4—C5	106.1 (2)
C1—N2—C3	111.6 (2)	O1—C4—H4A	110.5
O2—N2—C3	125.7 (2)	C5—C4—H4A	110.5
N1—C1—N2	103.6 (2)	O1—C4—H4B	110.5
N1—C1—S1	129.23 (19)	C5—C4—H4B	110.5
N2—C1—S1	127.1 (2)	H4A—C4—H4B	108.7
C2—C3—N2	106.4 (2)	C14—C13—C12	120.0 (3)
C2—C3—H3	126.8	C14—C13—H13	120.0
N2—C3—H3	126.8	C12—C13—H13	120.0
C17—C12—C13	119.3 (3)	S1—C18—H18A	109.5
C17—C12—C11	121.2 (2)	S1—C18—H18B	109.5
C13—C12—C11	119.4 (2)	H18A—C18—H18B	109.5
C8—C9—C10	120.4 (3)	S1—C18—H18C	109.5
C8—C9—H9	119.8	H18A—C18—H18C	109.5
C10—C9—H9	119.8	H18B—C18—H18C	109.5
C9—C10—C5	120.1 (3)	C15—C14—C13	120.5 (3)
C9—C10—H10	120.0	C15—C14—H14	119.8
C5—C10—H10	120.0	C13—C14—H14	119.8
C6—C5—C10	119.1 (2)	C15—C16—C17	120.3 (3)
C6—C5—C4	120.0 (3)	C15—C16—H16	119.9
C10—C5—C4	120.9 (3)	C17—C16—H16	119.9
N1—O1—C4—C5	-174.2 (2)	N2—O2—C11—C12	95.5 (2)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ F2A <sup>i</sup>	0.95	2.28	3.200 (13)	162
C2—H2 $\cdots$ F3B <sup>i</sup>	0.95	2.55	3.302 (14)	136
C2—H2 $\cdots$ F2C <sup>i</sup>	0.95	2.07	2.936 (10)	150
C4—H4B $\cdots$ F2B	0.99	2.52	3.472 (17)	162
C4—H4A $\cdots$ F3B <sup>i</sup>	0.99	2.50	3.183 (13)	126
C4—H4A $\cdots$ F2C <sup>i</sup>	0.99	2.56	3.39 (3)	141
C4—H4B $\cdots$ F4C	0.99	2.61	3.522 (19)	153
C8—H8 $\cdots$ F1 <sup>ii</sup>	0.95	2.54	3.317 (4)	139
C10—H10 $\cdots$ F3B <sup>i</sup>	0.95	2.46	3.282 (12)	145
C11—H11A $\cdots$ F3A <sup>iii</sup>	0.99	2.27	3.247 (13)	167

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C11—H11A···F3C <sup>ii</sup>	0.99	2.40	3.279 (15)	148
C18—H18C···F3A <sup>iii</sup>	0.98	2.62	3.409 (14)	138

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