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Hydroflumethiazide dimethyl sulfoxide disolvate

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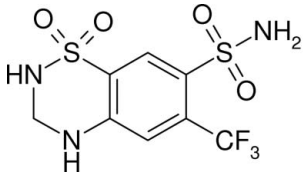
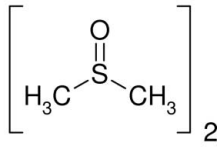
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.040; wR factor = 0.097; data-to-parameter ratio = 14.7.

Hydroflumethiazide forms a 1:2 solvate with dimethyl sulfoxide [systematic name: 3,4-dihydro-6-(trifluoromethyl)-2*H*-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide dimethyl sulfoxide disolvate], $C_8H_8F_3N_3O_4S_2\cdot 2C_2H_6OS$. The compound crystallizes with two molecules of solvent and one molecule of hydroflumethiazide in the asymmetric unit and displays an extensive network of hydrogen bonds. One solvent molecule is disordered over two positions, with site occupancy factors 0.57 (1) and 0.43 (1).

Related literature

For details of the experimental methods used to obtain this form of the title compound, see: Florence *et al.* (2003, 2006). For the crystal structures of hydroflumethiazide and of polymorphs and solvates of the related thiazide compounds chlorothiazide and hydrochlorothiazide, see: Florence *et al.* (2003), Fernandes *et al.* (2007); Johnston *et al.* (2007). For other related literature, see: Etter (1990).





Experimental

Crystal data

$C_8H_8F_3N_3O_4S_2\cdot 2C_2H_6OS$
M_r = 487.55
Monoclinic, $P2_1/c$
a = 5.5570 (1) Å
b = 20.8433 (4) Å
c = 17.4142 (3) Å
β = 93.540 (2)°
V = 2013.17 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 150 (2) K
0.30 × 0.04 × 0.04 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.917, T_{max} = 1.000 (expected range = 0.897–0.979)
20791 measured reflections
4097 independent reflections
3125 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.097
S = 1.04
4097 reflections
279 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H2···O5	0.87 (2)	1.98 (2)	2.837 (3)	170 (2)
N3—H3···O3^{i}	0.869 (19)	2.383 (17)	3.158 (3)	149 (2)
N1—H7···O6^{ii}	0.88	2.12	2.836 (3)	139
N2—H8···O6^{iii}	0.87 (2)	2.03 (2)	2.880 (3)	166 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003), *ORTEP-3* (Farrugia, 1997) and *Cerius*^{2} (Accelrys, 2001); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004) and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2189).

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supplementary materials

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Hydroflumethiazide dimethyl sulfoxide disolvate

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Comment

Hydroflumethiazide (HFMT) is a thiazide drug that is indicated in the management of hypertension and is known to crystallize in at least one non-solvated form (Florence *et al.*, 2003). This work forms part of a wider investigation that couples automated parallel crystallization (Florence *et al.*, 2006) with crystal structure prediction methodology to investigate the basic science underlying solid-state diversity in a range of thiazide diuretic compounds (Johnston *et al.*, 2007, Fernandes *et al.*, 2007). The sample was identified as a novel form using multi-sample foil transmission X-ray powder diffraction analysis (Florence *et al.*, 2003). Subsequent manual recrystallization from a saturated dimethyl sulfoxide solution (DMSO) by slow evaporation at 278 K yielded samples of the title compound suitable for single-crystal X-ray diffraction at 150 K (Fig. 1). The compound crystallizes with one molecule of HFMT and two molecules of DMSO in the asymmetric unit. One of the solvent molecules (residue C) is disordered over two sites with 0.43 (1) and 0.57 (1) occupancy, respectively.

The structure contains four N—H···O bonds (Table 1), with all available hydrogen-bond donors in HFMT forming contacts to adjactent sulfinyl O-atoms of DMSO. Contacts 2, 3 and 4 combine to create an $R_3^2(18)$ hydrogen-bonded motif (Etter, 1990) between HFMT and DMSO residue B, whilst contact 1 connects residue C to HFMT (Fig. 2).

Experimental

The compound was sourced from Sigma–Aldrich and a single-crystal sample of the title compound was recrystallized from a saturated dimethyl sulfoxide solution by isothermal solvent evaporation at room temperature.

Refinement

All non-hydrogen atoms were identified by direct methods and the positions of all the hydrogen atoms were obtained from the use of difference Fourier maps. In the final refinement, all hydrogen atoms were constrained to geometrically sensible positions with a riding model, except for H2, H3 and H8 which were allowed to refine subject to a distance restraint.

Figures

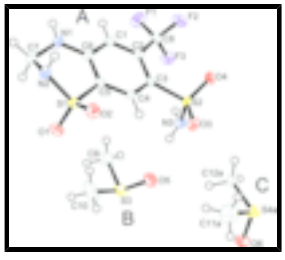

Fig. 1. The asymmetric unit of the title compound, showing 50% probablility displacement ellipsoids. Minor occupancy disordered atomic sites (residue C) have been omitted for clarity.

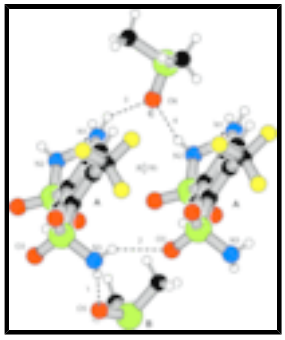

Fig. 2. The $R_3^2(18)$ hydrogen-bond motif in the title compound, involving HFMT and solvent residue C. Hydrogen bond 1 (Table 1) connects solvent residue B to HFMT. Minor disorder components have been omitted for clarity.

3,4-dihydro-6-(trifluoromethyl)-2*H*-1,2,4-benzothiadiazine-7- sulfonamide 1,1-dioxide dimethyl sulfoxide disolvate

Crystal data

$C_8H_8F_3N_3O_4S_2·2C_2H_6OS$	F_{000} = 1008
M_r = 487.55	D_x = 1.609 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8339 reflections
a = 5.55700 (10) Å	θ = 2.5–28.6º
b = 20.8433 (4) Å	μ = 0.53 mm^{-1}
c = 17.4142 (3) Å	T = 150 (2) K
β = 93.540 (2)º	Needle, colourless
V = 2013.17 (6) Å^3	0.30 × 0.04 × 0.04 mm
Z = 4	

Data collection

Oxford Diffraction Gemini diffractometer	4097 independent reflections
Radiation source: Enhance (Mo) X-ray source	3125 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 150(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	h = −6→6
T_{min} = 0.917, T_{max} = 1.000	k = −25→26
20791 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.097	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.661P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
4097 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
279 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	−0.01352 (11)	0.13727 (3)	0.55321 (3)	0.01901 (15)	
S2	0.35866 (11)	0.10571 (3)	0.84249 (3)	0.01901 (15)	
S3	0.60374 (14)	−0.07563 (3)	0.67961 (4)	0.03297 (19)	
F3	0.8236 (3)	0.18575 (7)	0.84137 (8)	0.0287 (4)	
F2	0.5879 (3)	0.26592 (7)	0.85879 (9)	0.0324 (4)	
O3	0.1426 (3)	0.06775 (8)	0.83638 (10)	0.0239 (4)	
F1	0.8528 (3)	0.27104 (8)	0.77485 (9)	0.0373 (4)	
O4	0.4004 (3)	0.14679 (8)	0.90741 (9)	0.0255 (4)	
O6	0.2205 (3)	−0.18457 (9)	0.94408 (11)	0.0285 (4)	
O1	0.0979 (3)	0.08578 (8)	0.51422 (10)	0.0263 (4)	
O2	−0.2453 (3)	0.12674 (9)	0.58203 (10)	0.0260 (4)	
O5	0.4708 (4)	−0.05271 (10)	0.74696 (11)	0.0379 (5)	
N1	0.3378 (4)	0.24697 (11)	0.54436 (12)	0.0240 (5)	
H7	0.4192	0.2829	0.5406	0.036*	
N2	−0.0319 (4)	0.19850 (10)	0.49524 (12)	0.0229 (5)	
N3	0.5777 (4)	0.05525 (11)	0.84224 (13)	0.0220 (5)	
C2	0.5116 (4)	0.20571 (11)	0.74488 (14)	0.0186 (5)	
C6	0.3410 (4)	0.21632 (12)	0.61364 (14)	0.0186 (5)	
C3	0.3592 (4)	0.15283 (11)	0.75733 (13)	0.0178 (5)	
C4	0.1986 (4)	0.13402 (11)	0.69812 (13)	0.0180 (5)	
H4	0.0920	0.0994	0.7061	0.027*	
C8	0.6924 (5)	0.23187 (13)	0.80502 (14)	0.0237 (6)	
C7	0.2046 (5)	0.22208 (13)	0.47697 (14)	0.0265 (6)	
H6	0.2971	0.1867	0.4549	0.040*	
H5	0.1848	0.2564	0.4378	0.040*	

C5	0.1887 (4)	0.16436 (12)	0.62726 (13)	0.0178 (5)	
C1	0.4980 (4)	0.23682 (12)	0.67517 (14)	0.0206 (5)	
H1	0.5975	0.2732	0.6684	0.031*	
C9	0.8253 (6)	−0.01685 (16)	0.66462 (18)	0.0431 (8)	
H9A	0.9498	−0.0183	0.7070	0.065*	
H9B	0.7502	0.0257	0.6626	0.065*	
H9C	0.8989	−0.0254	0.6159	0.065*	
C10	0.4173 (6)	−0.0605 (2)	0.59702 (18)	0.0577 (11)	
H10A	0.2706	−0.0864	0.5983	0.087*	
H10B	0.5028	−0.0717	0.5513	0.087*	
H10C	0.3742	−0.0149	0.5952	0.087*	
S4A	0.1219 (17)	−0.1206 (5)	0.9641 (6)	0.0344 (13)	0.432 (13)
C11A	−0.0889 (18)	−0.1033 (5)	0.8846 (7)	0.058 (3)*	0.432 (13)
H11A	−0.1920	−0.1408	0.8739	0.088*	0.432 (13)
H11B	−0.0009	−0.0932	0.8390	0.088*	0.432 (13)
H11C	−0.1890	−0.0666	0.8974	0.088*	0.432 (13)
C12A	0.3508 (16)	−0.0662 (3)	0.9396 (4)	0.0231 (19)*	0.432 (13)
H12A	0.4946	−0.0726	0.9742	0.035*	0.432 (13)
H12B	0.2929	−0.0221	0.9447	0.035*	0.432 (13)
H12C	0.3913	−0.0738	0.8864	0.035*	0.432 (13)
S4B	0.0685 (12)	−0.1247 (4)	0.9465 (4)	0.0275 (8)	0.568 (13)
C12B	0.2631 (15)	−0.0585 (3)	0.9532 (4)	0.0408 (18)*	0.568 (13)
H12D	0.3652	−0.0613	1.0010	0.061*	0.568 (13)
H12E	0.1683	−0.0189	0.9531	0.061*	0.568 (13)
H12F	0.3648	−0.0585	0.9092	0.061*	0.568 (13)
C11B	−0.0441 (11)	−0.1112 (3)	0.8491 (4)	0.0373 (18)*	0.568 (13)
H11D	−0.1557	−0.1458	0.8330	0.056*	0.568 (13)
H11E	0.0908	−0.1106	0.8154	0.056*	0.568 (13)
H11F	−0.1288	−0.0700	0.8456	0.056*	0.568 (13)
H3	0.716 (3)	0.0747 (12)	0.8421 (16)	0.031 (8)*	
H2	0.552 (5)	0.0249 (10)	0.8088 (13)	0.032 (8)*	
H8	−0.110 (4)	0.2296 (9)	0.5158 (15)	0.029 (8)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0192 (3)	0.0192 (3)	0.0183 (3)	−0.0019 (3)	−0.0008 (2)	−0.0012 (2)
S2	0.0203 (3)	0.0196 (3)	0.0173 (3)	0.0028 (3)	0.0026 (2)	0.0030 (2)
S3	0.0345 (4)	0.0281 (4)	0.0365 (4)	−0.0027 (3)	0.0034 (3)	−0.0094 (3)
F3	0.0234 (8)	0.0303 (9)	0.0310 (9)	0.0029 (7)	−0.0076 (7)	0.0019 (7)
F2	0.0369 (9)	0.0280 (9)	0.0314 (9)	0.0029 (7)	−0.0043 (7)	−0.0111 (7)
O3	0.0211 (9)	0.0261 (10)	0.0246 (10)	0.0004 (8)	0.0035 (8)	0.0072 (7)
F1	0.0321 (9)	0.0418 (10)	0.0367 (9)	−0.0197 (8)	−0.0074 (7)	0.0067 (8)
O4	0.0350 (11)	0.0257 (10)	0.0160 (9)	0.0040 (8)	0.0028 (8)	0.0001 (7)
O6	0.0254 (10)	0.0231 (10)	0.0365 (11)	0.0061 (8)	−0.0002 (8)	−0.0009 (8)
O1	0.0286 (10)	0.0236 (10)	0.0266 (10)	0.0011 (8)	−0.0002 (8)	−0.0065 (8)
O2	0.0182 (9)	0.0322 (11)	0.0274 (10)	−0.0031 (8)	0.0002 (8)	−0.0016 (8)
O5	0.0405 (12)	0.0409 (13)	0.0332 (11)	−0.0095 (10)	0.0097 (9)	−0.0107 (9)

N1	0.0244 (12)	0.0249 (12)	0.0222 (11)	−0.0069 (9)	−0.0021 (9)	0.0078 (9)
N2	0.0260 (12)	0.0224 (12)	0.0198 (11)	−0.0015 (10)	−0.0034 (9)	0.0014 (9)
N3	0.0199 (12)	0.0197 (12)	0.0261 (12)	0.0012 (10)	−0.0012 (10)	0.0012 (9)
C2	0.0161 (12)	0.0185 (13)	0.0210 (13)	0.0006 (10)	−0.0002 (10)	−0.0013 (10)
C6	0.0161 (12)	0.0200 (13)	0.0198 (12)	0.0024 (10)	0.0019 (10)	0.0010 (10)
C3	0.0192 (13)	0.0176 (13)	0.0166 (12)	0.0044 (10)	0.0027 (10)	0.0023 (9)
C4	0.0186 (12)	0.0142 (12)	0.0215 (12)	−0.0014 (10)	0.0032 (10)	−0.0010 (10)
C8	0.0241 (14)	0.0235 (14)	0.0230 (14)	−0.0021 (11)	−0.0027 (11)	0.0007 (11)
C7	0.0339 (15)	0.0263 (15)	0.0191 (13)	−0.0052 (12)	0.0005 (11)	0.0034 (11)
C5	0.0165 (12)	0.0202 (13)	0.0166 (12)	0.0013 (10)	0.0004 (10)	−0.0016 (10)
C1	0.0193 (13)	0.0176 (13)	0.0249 (13)	−0.0038 (10)	0.0017 (10)	0.0016 (10)
C9	0.0430 (19)	0.046 (2)	0.0406 (18)	−0.0100 (15)	0.0059 (15)	−0.0059 (15)
C10	0.0355 (19)	0.105 (3)	0.0318 (18)	0.0104 (19)	−0.0032 (15)	−0.0200 (19)
S4A	0.036 (3)	0.0231 (16)	0.045 (4)	0.005 (2)	0.013 (2)	0.003 (2)
S4B	0.034 (2)	0.0217 (13)	0.0277 (19)	0.0071 (15)	0.0101 (13)	0.0032 (12)

Geometric parameters (Å, °)

S1—O2	1.4278 (17)	C3—C4	1.378 (3)
S1—O1	1.4310 (18)	C4—C5	1.385 (3)
S1—N2	1.627 (2)	C4—H4	0.9500
S1—C5	1.751 (2)	C7—H6	0.9900
S2—O4	1.4258 (18)	C7—H5	0.9900
S2—O3	1.4361 (18)	C1—H1	0.9500
S2—N3	1.609 (2)	C9—H9A	0.9800
S2—C3	1.779 (2)	C9—H9B	0.9800
S3—O5	1.5023 (19)	C9—H9C	0.9800
S3—C10	1.748 (3)	C10—H10A	0.9800
S3—C9	1.768 (3)	C10—H10B	0.9800
F3—C8	1.341 (3)	C10—H10C	0.9800
F2—C8	1.336 (3)	S4A—C12A	1.776 (12)
F1—C8	1.340 (3)	S4A—C11A	1.795 (11)
O6—S4A	1.492 (10)	C11A—H11A	0.9800
O6—S4B	1.510 (8)	C11A—H11B	0.9800
N1—C6	1.364 (3)	C11A—H11C	0.9800
N1—C7	1.445 (3)	C12A—H12A	0.9800
N1—H7	0.8800	C12A—H12B	0.9800
N2—C7	1.457 (3)	C12A—H12C	0.9800
N2—H8	0.871 (10)	S4B—C12B	1.751 (9)
N3—H3	0.869 (10)	S4B—C11B	1.794 (8)
N3—H2	0.866 (10)	C12B—H12D	0.9800
C2—C1	1.374 (3)	C12B—H12E	0.9800
C2—C3	1.415 (3)	C12B—H12F	0.9800
C2—C8	1.508 (3)	C11B—H11D	0.9800
C6—C5	1.404 (3)	C11B—H11E	0.9800
C6—C1	1.406 (3)	C11B—H11F	0.9800
O2—S1—O1	118.53 (11)	N1—C7—N2	111.6 (2)
O2—S1—N2	108.38 (11)	N1—C7—H6	109.3
O1—S1—N2	107.84 (11)	N2—C7—H6	109.3

O2—S1—C5	110.04 (11)	N1—C7—H5	109.3
O1—S1—C5	108.33 (11)	N2—C7—H5	109.3
N2—S1—C5	102.52 (12)	H6—C7—H5	108.0
O4—S2—O3	118.94 (10)	C4—C5—C6	120.8 (2)
O4—S2—N3	107.98 (12)	C4—C5—S1	119.82 (19)
O3—S2—N3	105.59 (11)	C6—C5—S1	119.39 (18)
O4—S2—C3	108.71 (11)	C2—C1—C6	121.8 (2)
O3—S2—C3	106.67 (11)	C2—C1—H1	119.1
N3—S2—C3	108.57 (11)	C6—C1—H1	119.1
O5—S3—C10	106.85 (14)	S3—C9—H9A	109.5
O5—S3—C9	105.99 (13)	S3—C9—H9B	109.5
C10—S3—C9	97.83 (18)	H9A—C9—H9B	109.5
C6—N1—C7	121.9 (2)	S3—C9—H9C	109.5
C6—N1—H7	119.0	H9A—C9—H9C	109.5
C7—N1—H7	119.0	H9B—C9—H9C	109.5
C7—N2—S1	112.16 (17)	S3—C10—H10A	109.5
C7—N2—H8	108.6 (18)	S3—C10—H10B	109.5
S1—N2—H8	110.1 (19)	H10A—C10—H10B	109.5
S2—N3—H3	111.4 (19)	S3—C10—H10C	109.5
S2—N3—H2	113 (2)	H10A—C10—H10C	109.5
H3—N3—H2	117 (3)	H10B—C10—H10C	109.5
C1—C2—C3	120.2 (2)	O6—S4A—C12A	103.6 (6)
C1—C2—C8	116.2 (2)	O6—S4A—C11A	103.3 (5)
C3—C2—C8	123.7 (2)	C12A—S4A—C11A	97.5 (6)
N1—C6—C5	122.4 (2)	O6—S4B—C12B	108.0 (4)
N1—C6—C1	120.4 (2)	O6—S4B—C11B	105.4 (4)
C5—C6—C1	117.3 (2)	C12B—S4B—C11B	96.7 (5)
C4—C3—C2	118.2 (2)	S4B—C12B—H12D	109.5
C4—C3—S2	115.61 (18)	S4B—C12B—H12E	109.5
C2—C3—S2	126.14 (19)	H12D—C12B—H12E	109.5
C3—C4—C5	121.7 (2)	S4B—C12B—H12F	109.5
C3—C4—H4	119.2	H12D—C12B—H12F	109.5
C5—C4—H4	119.2	H12E—C12B—H12F	109.5
F2—C8—F1	106.2 (2)	S4B—C11B—H11D	109.5
F2—C8—F3	107.3 (2)	S4B—C11B—H11E	109.5
F1—C8—F3	105.5 (2)	H11D—C11B—H11E	109.5
F2—C8—C2	112.3 (2)	S4B—C11B—H11F	109.5
F1—C8—C2	112.3 (2)	H11D—C11B—H11F	109.5
F3—C8—C2	112.8 (2)	H11E—C11B—H11F	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H2···O5	0.87 (2)	1.98 (2)	2.837 (3)	170 (2)
N3—H3···O3^{i}	0.869 (19)	2.383 (17)	3.158 (3)	149 (2)
N1—H7···O6^{ii}	0.88	2.12	2.836 (3)	139
N2—H8···O6^{iii}	0.87 (2)	2.03 (2)	2.880 (3)	166 (2)

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

Fig. 1

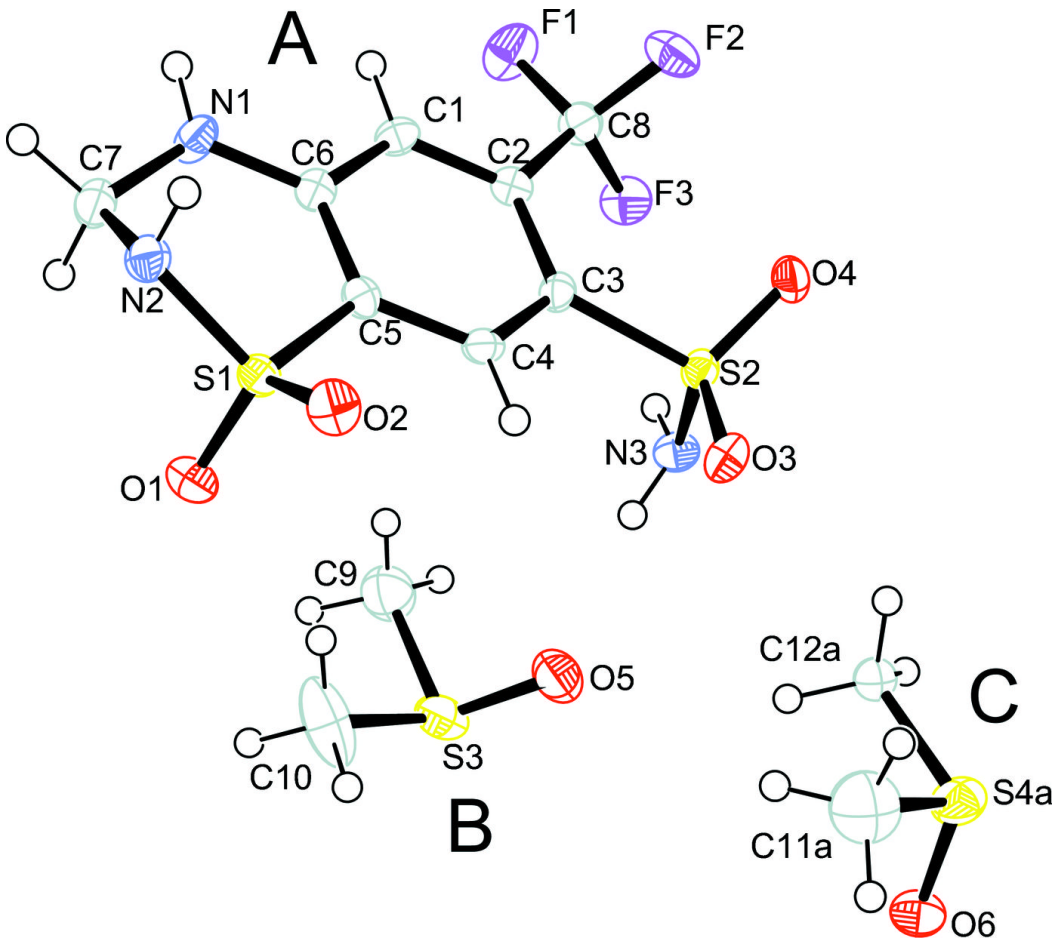
A
F1
F2
N1
C1
C8
C7
C6
C2
F3
O4
C3
N2
C5
C4
S1
S2
O2
N3
O3
O1
C9
O5
S3
C10
B
C12a
C
S4a
C11a
O6

Fig. 2