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Anilinium hydrogen sulfate

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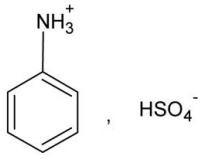
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.117; data-to-parameter ratio = 21.2.

The asymmetric unit of the title compound, $C_6H_8N^+\cdot HSO_4^-$, contains two cations and two anions which are linked to each other through N—H···O hydrogen bonds, formed by all H atoms covalently bonded to the N atoms. In addition, strong O—H···O anion–anion hydrogen-bond interactions are also observed.

Related literature

For hydrogen bonding, see: Zimmerman & Corbin (2000); Brunsveld *et al.* (2001); Desiraju (2002); Desiraju & Steiner (1999); Steiner (2002); Etter *et al.* (1990); Bernstein *et al.* (1995). For related structures, see: Benali-Cherif, Boussekine *et al.* (2009); Messai *et al.* (2009); Benali-Cherif, Falek *et al.* (2009); Rademeyer (2004); Jayaraman *et al.* (2002); Smith *et al.* (2004); Paixão *et al.* (2000).



Experimental

Crystal data

$C_6H_8N^+\cdot HSO_4^-$
M_r = 191.20
Orthorhombic, $Pca2_1$
a = 14.3201 (2) Å
b = 9.0891 (3) Å
c = 12.8771 (2) Å
V = 1676.04 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 293 K
0.2 × 0.15 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
16963 measured reflections
4641 independent reflections
3108 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.02
4641 reflections
219 parameters
1 restraint
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), 2096 Friedel pairs
Flack parameter: 0.08 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H11···O1A^{i}	0.89	1.95	2.821 (2)	167
N1A—H22···O3B	0.89	1.95	2.817 (4)	163
N1A—H33···O2B^{iii}	0.89	2.01	2.884 (3)	169
N1B—H1···O1B^{ii}	0.89	1.94	2.828 (3)	175
N1B—H2···O3A^{ii}	0.89	2.05	2.867 (3)	153
N1B—H3···O1A	0.89	2.58	3.069 (3)	115
N1B—H3···O2A	0.89	2.03	2.916 (3)	175
O4A—H4···O3B	0.82	1.79	2.603 (4)	175
O4B—H44···O3A^{i}	0.82	1.84	2.635 (4)	163

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

Data collection: *KappaCCD Server Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-32 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2534).

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supporting information

Acta Cryst. (2010). E**66**, o595–o596 [doi:10.1107/S1600536810004782]

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S1. Comment

The main purpose of this structural study was a determination of the arrangement of the cations and anions which are held together by two-dimensional hydrogen-bond networks.

Hydrogen bonding is one of the most versatile noncovalent forces in supramolecular chemistry and crystal engineering (Zimmerman & Corbin, 2000; Brunsveld *et al.*, 2001; Desiraju, 2002). Therefore, in the past decades assessment of discrete hydrogen bonding patterns had received great attention (Steiner, 2002; Desiraju & Steiner, 1999) because of its widespread occurrence in biological systems.

The aim of this paper is to discuss hydrogen patterns assuring the connection between anilinium and hydrogensulfate entities and to establish their different graph-set motifs (Bernstein *et al.*, 1995).

Bis(anilinium hydrogensulfate) is one of the hybrid compounds, rich in H-bonds (Benali-Cherif, Boussekine, *et al.*, 2009; Messai *et al.*, 2009; Benali-Cherif, Falek, *et al.*, 2009), which could have potential importance in constructing sophisticated assemblies from discrete ionic or molecular building blocks due to the strength and the directionality of hydrogen bonds (Steiner *et al.* 2002, Jayaraman *et al.*, 2002).

Recently, similar structures containing anilinium cations have been reported. Among examples, can be named the folowing ones: anilinium nitrate (Rademeyer, 2004), anilinium picrate (Smith *et al.*, 2004), anilinium hydrogenphosphite and anilinium hydrogenoxalate hemihydrate(Paixão *et al.*, 2000).

The structure of (I) may be described as formed by alternating sheets of cations and anions (Fig. 2) which are held together with four and five-centered N—H···O H-bonds to form $C_4^4(10)$ infinite chains running through the c direction. Moreover, strong O—H···O hydrogen bonds observed between bisulfate anions generate $C_2^2(8)$ chains in the *a* axis direction. The infinite chains resulting from anion-anion and anion-cation interactions can be described as zigzag layers parallel to the (*ac*) plane (Fig. 3). The crossing of these chains builds up different rings with $R_3^3(10)$ and $R_5^4(16)$ graph set motifs (Fig. 3) (Etter *et al.*, 1990; Bernstein *et al.*, 1995).

S2. Experimental

Single crystals of the title compound are prepared by slow evaporation at room temperature of an aqueous solution of aniline and sulfuric acid.

S3. Refinement

The title compound crystallizes in the centrosymmetric space group P c a 2_1. All non-H atoms were refined with anisotropic atomic displacement parameters. H atoms were located from Fourier difference maps and treated as riding with C—H = 0.93 Å, N—H = 0.89 Å and O—H = 0.82 Å. Their isotropic displacement parameters were set equal to 1.2Ueq (C) and 1.5Ueq (N, O).

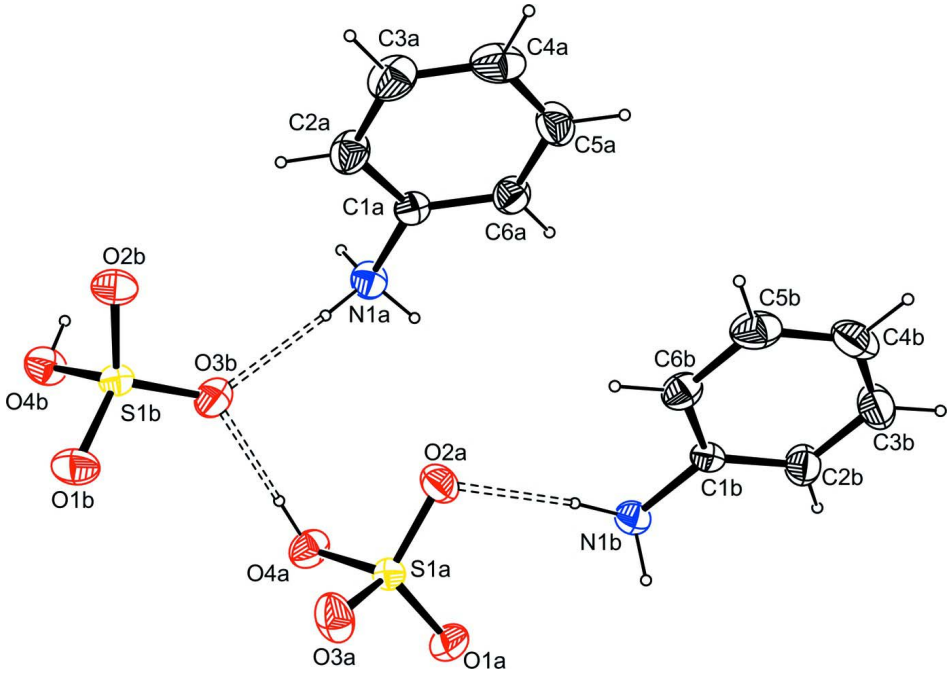

Figure 1

ORTEP view of the asymmetric unit of (I) showing 10% probability displacement ellipsoids.

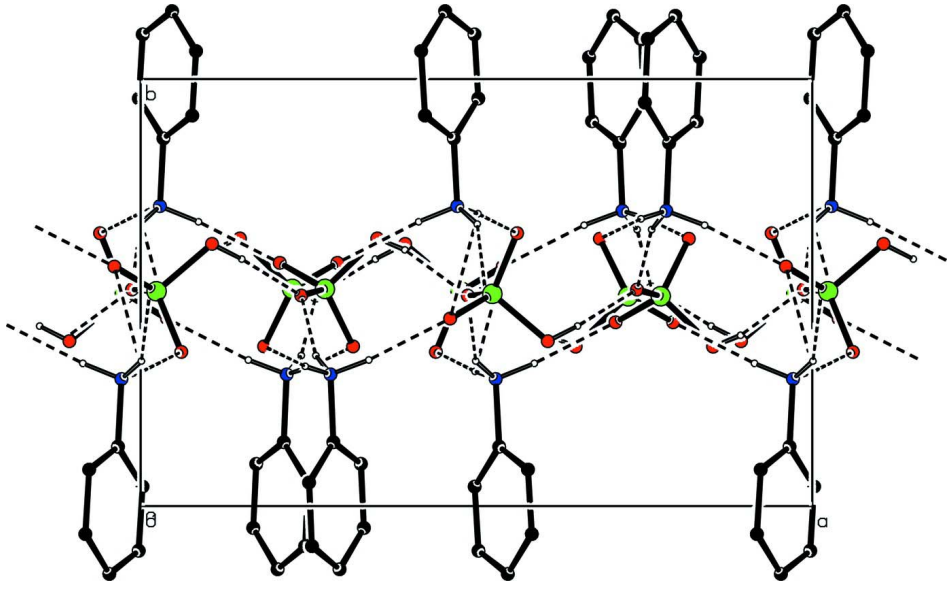

Figure 2

Alternating cationic and anionc layers visualized through the (001) plane.

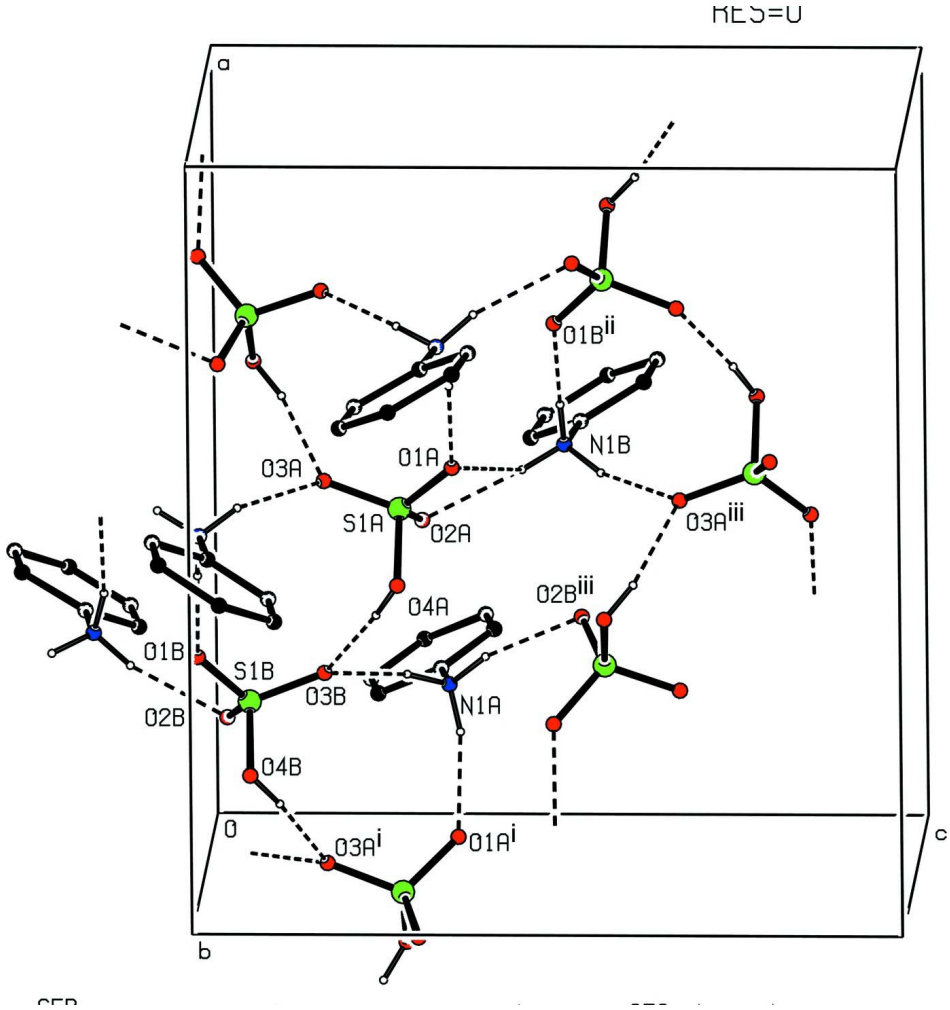

Figure 3

Intermolecular hydrogen bonding patterns running parallel to (*bc*) plane. H atoms not involved in hydrogen bondings have been omitted for clarity. [Symmetry codes: (i) *x*-1/2, -*y*+1, *z*; (ii) -*x*+1, -*y*+1, *z*+1/2; (iii) -*x*+1/2, *y*, *z*+1/2.

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Crystal data

$C_6H_8N^+\cdot HSO_4^-$
M_r = 191.20
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
a = 14.3201 (2) Å
b = 9.0891 (3) Å
c = 12.8771 (2) Å
V = 1676.04 (7) Å^3
Z = 8
F(000) = 800
D_x = 1.516 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 16963 reflections
θ = 2.7–30.0°
μ = 0.36 mm^{-1}
T = 293 K
Prism, colourless
0.2 × 0.15 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega - \theta$ scans
16963 measured reflections
4641 independent reflections
3108 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.7°$
$h = -19 \rightarrow 17$
$k = -9 \rightarrow 12$
$l = -18 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.117$
$S = 1.02$
4641 reflections
219 parameters
1 restraint
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 not refined
$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.1354P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}
Absolute structure: Flack (1983), 2096 Friedel pairs
Absolute structure parameter: 0.08 (9)

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.

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 $F^2 > \sigma(F^2)$ 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}
N1A	0.21732 (15)	0.3085 (2)	0.3390 (2)	0.0432 (5)
H22	0.2392	0.3525	0.2823	0.065*
H33	0.2550	0.3273	0.3924	0.065*
H11	0.1603	0.3422	0.3530	0.065*
C1A	0.21307 (19)	0.1496 (3)	0.3217 (3)	0.0363 (7)
C2A	0.1721 (3)	0.0988 (4)	0.2311 (3)	0.0531 (8)
H2A	0.1482	0.1641	0.1823	0.064*
C3A	0.1676 (3)	−0.0512 (4)	0.2153 (3)	0.0626 (10)
H3A	0.1398	−0.0875	0.1553	0.075*
C4A	0.2039 (2)	−0.1480 (4)	0.2873 (4)	0.0640 (11)
H4A	0.2006	−0.2489	0.2760	0.077*
C5A	0.2449 (3)	−0.0940 (4)	0.3758 (3)	0.0555 (9)
H5A	0.2698	−0.1588	0.4243	0.067*
C6A	0.2493 (3)	0.0551 (4)	0.3931 (3)	0.0458 (7)
H6A	0.2770	0.0912	0.4533	0.055*

N1B	0.52868 (13)	0.2975 (2)	0.5035 (2)	0.0403 (5)
H1	0.5861	0.3342	0.4989	0.061*
H2	0.4989	0.3397	0.5564	0.061*
H3	0.4978	0.3154	0.4448	0.061*
C1B	0.53385 (18)	0.1390 (3)	0.5207 (2)	0.0330 (6)
C2B	0.5767 (2)	0.0855 (4)	0.6081 (3)	0.0498 (8)
H2B	0.6015	0.1493	0.6573	0.060*
C3B	0.5824 (3)	−0.0655 (4)	0.6217 (4)	0.0622 (10)
H3B	0.6104	−0.1037	0.6810	0.075*
C4B	0.5467 (3)	−0.1590 (4)	0.5479 (4)	0.0622 (11)
H4B	0.5521	−0.2602	0.5568	0.075*
C5B	0.5030 (3)	−0.1046 (4)	0.4610 (4)	0.0599 (11)
H5B	0.4775	−0.1685	0.4122	0.072*
C6B	0.4973 (3)	0.0456 (4)	0.4468 (3)	0.0453 (7)
H6B	0.4688	0.0836	0.3877	0.054*
S1A	0.47642 (6)	0.50293 (6)	0.27815 (5)	0.0354 (3)
O1A	0.53917 (14)	0.5609 (3)	0.3548 (2)	0.0588 (5)
O2A	0.43955 (15)	0.3610 (2)	0.30490 (17)	0.0501 (5)
O3A	0.5129 (3)	0.5072 (3)	0.1721 (3)	0.0610 (11)
O4A	0.39386 (13)	0.6139 (2)	0.27837 (19)	0.0492 (5)
H4	0.3495	0.5784	0.2468	0.074*
S1B	0.22562 (6)	0.50860 (7)	0.06533 (5)	0.0340 (3)
O1B	0.29288 (13)	0.5696 (2)	−0.00469 (18)	0.0543 (5)
O2B	0.18378 (13)	0.3739 (2)	0.02858 (18)	0.0477 (5)
O3B	0.2609 (3)	0.4930 (2)	0.1701 (3)	0.0570 (10)
O4B	0.14771 (13)	0.6268 (2)	0.0699 (2)	0.0493 (5)
H44	0.1067	0.6000	0.1100	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1A	0.0488 (13)	0.0354 (12)	0.0452 (12)	0.0039 (9)	−0.0019 (9)	−0.0050 (10)
C1A	0.0319 (14)	0.0339 (15)	0.0431 (16)	0.0026 (11)	0.0016 (12)	−0.0062 (12)
C2A	0.0594 (19)	0.0502 (19)	0.0496 (18)	0.0050 (16)	−0.0107 (17)	−0.0079 (17)
C3A	0.069 (2)	0.055 (2)	0.063 (3)	−0.001 (2)	−0.0126 (19)	−0.023 (2)
C4A	0.0542 (19)	0.0386 (19)	0.099 (3)	−0.0010 (14)	0.007 (2)	−0.022 (2)
C5A	0.0558 (18)	0.0426 (17)	0.068 (3)	0.0087 (16)	−0.0002 (19)	0.0097 (17)
C6A	0.0451 (15)	0.045 (2)	0.0471 (18)	−0.0003 (18)	−0.0043 (14)	−0.0026 (16)
N1B	0.0429 (11)	0.0348 (12)	0.0433 (11)	−0.0024 (9)	0.0007 (9)	−0.0008 (10)
C1B	0.0320 (14)	0.0303 (14)	0.0366 (15)	−0.0033 (10)	0.0044 (11)	0.0006 (11)
C2B	0.0532 (18)	0.0478 (18)	0.0483 (17)	0.0025 (15)	−0.0088 (16)	0.0018 (15)
C3B	0.062 (2)	0.058 (3)	0.067 (2)	0.008 (2)	0.003 (2)	0.024 (2)
C4B	0.0561 (19)	0.0345 (18)	0.096 (3)	−0.0007 (15)	0.021 (2)	0.0099 (19)
C5B	0.0511 (18)	0.045 (2)	0.084 (3)	−0.0072 (17)	0.004 (2)	−0.0201 (19)
C6B	0.0410 (15)	0.0461 (19)	0.0487 (19)	−0.0017 (18)	−0.0040 (14)	−0.0100 (17)
S1A	0.0319 (6)	0.0352 (5)	0.0392 (6)	−0.0012 (2)	−0.0005 (5)	0.0038 (2)
O1A	0.0503 (12)	0.0554 (14)	0.0705 (14)	−0.0116 (11)	−0.0226 (10)	0.0051 (12)
O2A	0.0625 (13)	0.0365 (11)	0.0514 (12)	−0.0065 (10)	−0.0036 (10)	0.0067 (8)

O3A	0.058 (2)	0.075 (2)	0.050 (2)	0.0183 (11)	0.0188 (19)	0.0205 (10)
O4A	0.0391 (10)	0.0430 (11)	0.0655 (13)	0.0065 (8)	−0.0047 (9)	−0.0081 (10)
S1B	0.0305 (6)	0.0341 (5)	0.0374 (5)	−0.0020 (2)	0.0013 (4)	−0.0020 (3)
O1B	0.0427 (11)	0.0621 (16)	0.0580 (13)	−0.0112 (10)	0.0141 (9)	0.0022 (12)
O2B	0.0499 (11)	0.0368 (10)	0.0564 (12)	−0.0074 (9)	0.0048 (9)	−0.0099 (9)
O3B	0.0476 (18)	0.073 (2)	0.050 (2)	−0.0086 (10)	−0.0119 (18)	0.0084 (10)
O4B	0.0470 (11)	0.0379 (11)	0.0630 (12)	0.0054 (9)	0.0082 (10)	0.0013 (10)

Geometric parameters (Å, º)

N1A—C1A	1.462 (4)	C1B—C6B	1.378 (4)
N1A—H22	0.8900	C2B—C3B	1.386 (6)
N1A—H33	0.8900	C2B—H2B	0.9300
N1A—H11	0.8900	C3B—C4B	1.373 (6)
C1A—C6A	1.361 (5)	C3B—H3B	0.9300
C1A—C2A	1.385 (5)	C4B—C5B	1.374 (6)
C2A—C3A	1.380 (5)	C4B—H4B	0.9300
C2A—H2A	0.9300	C5B—C6B	1.380 (4)
C3A—C4A	1.380 (6)	C5B—H5B	0.9300
C3A—H3A	0.9300	C6B—H6B	0.9300
C4A—C5A	1.372 (6)	S1A—O1A	1.435 (2)
C4A—H4A	0.9300	S1A—O2A	1.436 (2)
C5A—C6A	1.375 (4)	S1A—O3A	1.463 (4)
C5A—H5A	0.9300	S1A—O4A	1.554 (2)
C6A—H6A	0.9300	O4A—H4	0.8201
N1B—C1B	1.460 (3)	S1B—O1B	1.431 (2)
N1B—H1	0.8900	S1B—O2B	1.4430 (19)
N1B—H2	0.8900	S1B—O3B	1.448 (4)
N1B—H3	0.8900	S1B—O4B	1.550 (2)
C1B—C2B	1.371 (4)	O4B—H44	0.8200
C1A—N1A—H22	109.5	C2B—C1B—N1B	119.8 (3)
C1A—N1A—H33	109.5	C6B—C1B—N1B	119.0 (3)
H22—N1A—H33	109.5	C1B—C2B—C3B	118.8 (3)
C1A—N1A—H11	109.5	C1B—C2B—H2B	120.6
H22—N1A—H11	109.5	C3B—C2B—H2B	120.6
H33—N1A—H11	109.5	C4B—C3B—C2B	120.2 (3)
C6A—C1A—C2A	121.4 (3)	C4B—C3B—H3B	119.9
C6A—C1A—N1A	120.3 (3)	C2B—C3B—H3B	119.9
C2A—C1A—N1A	118.4 (3)	C3B—C4B—C5B	120.7 (4)
C3A—C2A—C1A	118.2 (3)	C3B—C4B—H4B	119.7
C3A—C2A—H2A	120.9	C5B—C4B—H4B	119.7
C1A—C2A—H2A	120.9	C4B—C5B—C6B	119.4 (3)
C2A—C3A—C4A	120.9 (3)	C4B—C5B—H5B	120.3
C2A—C3A—H3A	119.6	C6B—C5B—H5B	120.3
C4A—C3A—H3A	119.6	C1B—C6B—C5B	119.7 (3)
C5A—C4A—C3A	119.4 (3)	C1B—C6B—H6B	120.2
C5A—C4A—H4A	120.3	C5B—C6B—H6B	120.2

C3A—C4A—H4A	120.3	O1A—S1A—O2A	113.28 (16)
C4A—C5A—C6A	120.5 (3)	O1A—S1A—O3A	114.1 (2)
C4A—C5A—H5A	119.8	O2A—S1A—O3A	112.27 (15)
C6A—C5A—H5A	119.8	O1A—S1A—O4A	103.72 (14)
C1A—C6A—C5A	119.6 (3)	O2A—S1A—O4A	107.62 (12)
C1A—C6A—H6A	120.2	O3A—S1A—O4A	104.85 (16)
C5A—C6A—H6A	120.2	S1A—O4A—H4	109.5
C1B—N1B—H1	109.5	O1B—S1B—O2B	113.68 (16)
C1B—N1B—H2	109.5	O1B—S1B—O3B	113.0 (2)
H1—N1B—H2	109.5	O2B—S1B—O3B	111.55 (14)
C1B—N1B—H3	109.5	O1B—S1B—O4B	103.86 (13)
H1—N1B—H3	109.5	O2B—S1B—O4B	107.56 (12)
H2—N1B—H3	109.5	O3B—S1B—O4B	106.47 (17)
C2B—C1B—C6B	121.2 (3)	S1B—O4B—H44	109.5
C6A—C1A—C2A—C3A	0.9 (5)	C6B—C1B—C2B—C3B	−0.4 (4)
N1A—C1A—C2A—C3A	−179.6 (3)	N1B—C1B—C2B—C3B	−178.8 (3)
C1A—C2A—C3A—C4A	−0.7 (5)	C1B—C2B—C3B—C4B	0.9 (4)
C2A—C3A—C4A—C5A	0.0 (6)	C2B—C3B—C4B—C5B	−1.6 (5)
C3A—C4A—C5A—C6A	0.4 (6)	C3B—C4B—C5B—C6B	1.7 (6)
C2A—C1A—C6A—C5A	−0.4 (5)	C2B—C1B—C6B—C5B	0.5 (5)
N1A—C1A—C6A—C5A	−180.0 (3)	N1B—C1B—C6B—C5B	178.9 (3)
C4A—C5A—C6A—C1A	−0.2 (5)	C4B—C5B—C6B—C1B	−1.1 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H11···O1*A*^{i}	0.89	1.95	2.821 (2)	167
N1*B*—H2···O3*A*^{ii}	0.89	2.05	2.867 (3)	153
N1*A*—H33···O2*B*^{iii}	0.89	2.01	2.884 (3)	169
N1*B*—H3···O1*A*	0.89	2.58	3.069 (3)	115
N1*B*—H3···O2*A*	0.89	2.03	2.916 (3)	175
N1*A*—H22···O3*B*	0.89	1.95	2.817 (4)	163
O4*A*—H4···O3*B*	0.82	1.79	2.603 (4)	175
O4*B*—H44···O3*A*^{i}	0.82	1.84	2.635 (4)	163
N1*B*—H1···O1*B*^{ii}	0.89	1.94	2.828 (3)	175

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