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2-Nitro-*N*-(4-pyridinio)benzenesulfonamidate monohydrate

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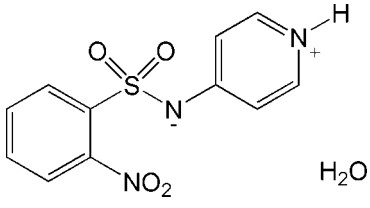
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.090; data-to-parameter ratio = 12.0.

The title compound, $C_{11}H_9N_3O_4S\cdot H_2O$, contains both an acid and a base centre and displays a zwitterionic structure. There are two independent molecules and two water molecules in the asymmetric unit. The dihedral angles between the benzene ring and the pyridinium ring are 109.7 (1) and 110.7 (1)°. The dihedral angles between the nitro group and the benzene ring are 116.1 (2) and 116.7 (1)°. The crystal structure is stabilized by N—H···O, O—H···N and O—H···O hydrogen bonds.

Related literature

For the uses of organic pyridinium salts, see: Damiano *et al.* (2007). For zwitterionic forms of *N*-arylbenzenesulfonamides, see: Li *et al.* (2007); Yu & Li (2007). For reference geometric data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_9N_3O_4S\cdot H_2O$
M_r = 297.29
Monoclinic, $P2_1$
a = 8.7206 (17) Å
b = 11.972 (2) Å
c = 12.743 (3) Å
β = 107.65 (3)°
V = 1267.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 113 (2) K
0.14 × 0.10 × 0.04 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.962, T_{max} = 0.989
10348 measured reflections
4633 independent reflections
3587 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.090
S = 1.03
4633 reflections
385 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), 1560 Friedel pairs
Flack parameter: 0.52 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O9	0.913 (10)	1.868 (12)	2.764 (3)	167 (3)
O9—H9A···O1	0.864 (10)	2.122 (11)	2.967 (3)	166 (3)
N1—H1A···O10^{i}	0.918 (10)	1.843 (11)	2.757 (3)	174 (4)
O9—H9B···N5^{ii}	0.867 (10)	2.043 (11)	2.901 (3)	170 (2)
O9—H9B···O6^{ii}	0.867 (10)	2.56 (2)	3.125 (3)	123 (2)
O10—H10A···O6^{iii}	0.867 (10)	2.051 (11)	2.914 (3)	174 (4)
O10—H10B···N2^{iv}	0.870 (10)	2.042 (12)	2.902 (3)	170 (3)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2431).

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Li, J.-S., Chen, L.-G., Zhang, Y.-Y., Xu, Y.-J., Deng, Y., Zeng, T. & Huang, P.-M. (2007). *J. Chem. Res.* pp. 350–352.
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supporting information

Acta Cryst. (2008). E**64**, o2277 [doi:10.1107/S1600536808035526]

2-Nitro-*N*-(4-pyridinio)benzenesulfonamidate monohydrate

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S1. Comment

Organic pyridinium salts have been widely used in the construction of supramolecular architectures (Damiano *et al.*, 2007). As part of our ongoing studies of supramolecular chemistry involving the pyridinium rings (Li *et al.*, 2007), the structure of the title compound was determined by X-ray diffraction. There are two independent molecules and two independent water molecules in the unit cell. In the cations of the title compound the short C—N distance [N2—C1 = 1.367 (3) Å and N5—C12 = 1.365 (3) Å] indicate the slight conjugation of the sulfonamide N with the pyridinium ring (Allen *et al.*, 1987).

The dihedral angles between the benzene ring and the pyridinium ring are 109.7 (1)° and 110.7 (1)° respectively. And the dihedral angles between the nitro group and the benzene ring are 116.1 (2)° and 116.7 (1)° respectively. The crystal structure is stabilized by N—H···O hydrogen bonds.

S2. Experimental

A solution of 2-nitrobenzenesulfonyl chloride (2.2 g, 10 mmol) in CH_2Cl_2 (10 ml) was added dropwise to a suspension of 4-aminopyridine (0.9 g, 10 mmol) in CH_2Cl_2 (10 ml) at room temperature with stirring. The reaction mixture was stirred overnight. The yellow solid obtained was washed with warm water to obtain the title compound in a yield of 55.7%. A colorless single crystal suitable for X-ray analysis was obtained by slow evaporation of an NaOH (10%) solution at room temperature over a period of a week.

S3. Refinement

The N-bound H atoms were located in a difference map and their coordinates were refined with U_{iso}(H) = 1.2U_{eq}(N). The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The Flack test results are ambiguous because of the presence of merohedral twin. The water O-bound H atoms were refined freely, but the O—H distances were restrained to 0.85 (1) Å, and the water HA···HB distance to 1.45 (1) Å.

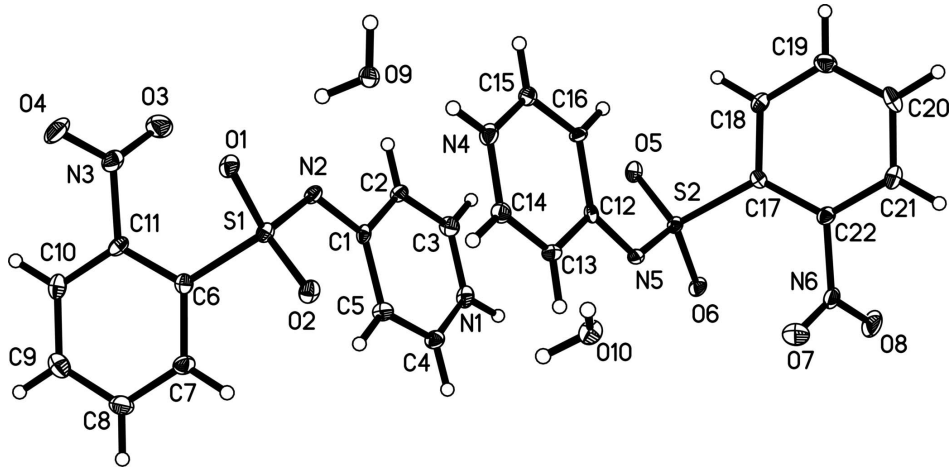

Figure 1

View of the molecule of title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level (arbitrary spheres for the H atoms).

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Crystal data

$C_{11}H_9N_3O_4S\cdot H_2O$
$M_r = 297.29$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 8.7206\ (17)$ Å
$b = 11.972\ (2)$ Å
$c = 12.743\ (3)$ Å
$\beta = 107.65\ (3)°$
$V = 1267.8\ (4)$ Å^3
$Z = 4$
$F(000) = 616$
$D_x = 1.557$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4439 reflections
$\theta = 2.4–27.5°$
$\mu = 0.28$ mm^{-1}
$T = 113$ K
Block, colourless
0.14 × 0.10 × 0.04 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: rotating anode
Confocal monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.962$, $T_{max} = 0.989$
10348 measured reflections
4633 independent reflections
3587 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
$h = -11\rightarrow11$
$k = -12\rightarrow15$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.090$
$S = 1.03$
4633 reflections
385 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.22$ e Å^{-3}

$\Delta\rho_{min} = -0.40$ e Å^{-3}

Absolute structure: Flack (1983), with how many Friedel pairs?
Absolute structure parameter: 0.52 (6)

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 $F^2 > \sigma(F^2)$ 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}
S1	0.54299 (7)	0.49945 (5)	0.75574 (5)	0.01423 (14)
S2	1.01577 (7)	0.25356 (5)	0.35546 (5)	0.01307 (14)
O1	0.36887 (19)	0.49815 (17)	0.72910 (14)	0.0177 (4)
O2	0.6116 (2)	0.59540 (15)	0.71745 (16)	0.0187 (4)
O3	0.4219 (3)	0.29003 (18)	0.87441 (18)	0.0318 (5)
O4	0.2777 (2)	0.4008 (2)	0.94108 (18)	0.0326 (5)
O5	0.9524 (2)	0.15286 (15)	0.38857 (15)	0.0165 (4)
O6	1.1904 (2)	0.26159 (18)	0.38501 (16)	0.0182 (4)
O7	1.1373 (3)	0.46983 (18)	0.24125 (19)	0.0334 (5)
O8	1.2807 (2)	0.3638 (2)	0.16880 (18)	0.0371 (6)
N1	1.0324 (3)	0.2999 (2)	0.67719 (19)	0.0185 (5)
N2	0.5920 (2)	0.38299 (18)	0.71702 (19)	0.0146 (5)
N3	0.4050 (3)	0.3727 (2)	0.9245 (2)	0.0217 (5)
N4	0.5077 (3)	0.4240 (2)	0.43389 (18)	0.0179 (5)
N5	0.9564 (2)	0.36491 (18)	0.39696 (18)	0.0141 (5)
N6	1.1564 (3)	0.3888 (2)	0.18846 (19)	0.0230 (6)
C1	0.7414 (3)	0.3615 (2)	0.7078 (2)	0.0132 (5)
C2	0.7644 (3)	0.2549 (2)	0.6690 (2)	0.0167 (5)
H2	0.6813	0.2029	0.6537	0.020*
C3	0.9100 (3)	0.2265 (2)	0.6532 (2)	0.0188 (6)
H3	0.9231	0.1563	0.6259	0.023*
C4	1.0168 (3)	0.4019 (2)	0.7153 (2)	0.0179 (6)
H4	1.1030	0.4513	0.7304	0.021*
C5	0.8752 (3)	0.4350 (2)	0.7325 (2)	0.0169 (6)
H5	0.8672	0.5058	0.7604	0.020*
C6	0.6158 (3)	0.5053 (3)	0.9027 (2)	0.0148 (5)
C7	0.7441 (3)	0.5753 (2)	0.9531 (2)	0.0189 (6)
H7	0.7936	0.6156	0.9100	0.023*
C8	0.7996 (3)	0.5858 (2)	1.0674 (2)	0.0240 (6)
H8	0.8857	0.6329	1.0999	0.029*
C9	0.7271 (3)	0.5264 (3)	1.1326 (2)	0.0245 (7)
H9	0.7656	0.5325	1.2089	0.029*

C10	0.5978 (3)	0.4582 (2)	1.0843 (2)	0.0208 (6)
H10	0.5469	0.4197	1.1277	0.025*
C11	0.5441 (3)	0.4472 (2)	0.9712 (2)	0.0162 (6)
C12	0.8049 (3)	0.3782 (2)	0.4049 (2)	0.0120 (5)
C13	0.7734 (3)	0.4806 (2)	0.4510 (2)	0.0163 (6)
H13	0.8534	0.5347	0.4722	0.020*
C14	0.6264 (3)	0.4998 (2)	0.4642 (2)	0.0181 (5)
H14	0.6078	0.5669	0.4949	0.022*
C15	0.5302 (3)	0.3265 (2)	0.3884 (2)	0.0165 (5)
H15	0.4464	0.2752	0.3672	0.020*
C16	0.6767 (3)	0.3014 (2)	0.3725 (2)	0.0136 (5)
H16	0.6905	0.2339	0.3405	0.016*
C17	0.9459 (3)	0.2526 (2)	0.2084 (2)	0.0145 (5)
C18	0.8167 (3)	0.1850 (2)	0.1552 (2)	0.0179 (6)
H18	0.7672	0.1423	0.1967	0.021*
C19	0.7603 (3)	0.1799 (2)	0.0417 (2)	0.0229 (6)
H19	0.6723	0.1349	0.0080	0.027*
C20	0.8324 (3)	0.2406 (3)	−0.0223 (2)	0.0245 (7)
H20	0.7933	0.2365	−0.0987	0.029*
C21	0.9631 (3)	0.3074 (2)	0.0276 (2)	0.0195 (6)
H21	1.0141	0.3476	−0.0146	0.023*
C22	1.0173 (3)	0.3137 (2)	0.1415 (2)	0.0157 (6)
O9	0.2408 (2)	0.50194 (18)	0.48520 (16)	0.0183 (4)
O10	0.6923 (2)	0.74683 (18)	0.37557 (18)	0.0203 (4)
H1A	1.127 (3)	0.280 (3)	0.665 (3)	0.054 (11)*
H4A	0.411 (2)	0.441 (2)	0.444 (2)	0.021 (8)*
H9A	0.260 (3)	0.500 (3)	0.5558 (8)	0.047 (11)*
H9B	0.160 (2)	0.460 (2)	0.4517 (18)	0.024 (9)*
H10A	0.719 (4)	0.751 (4)	0.4468 (8)	0.11 (2)*
H10B	0.601 (2)	0.780 (3)	0.346 (2)	0.034 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0127 (3)	0.0152 (3)	0.0156 (3)	0.0016 (3)	0.0055 (2)	0.0026 (3)
S2	0.0098 (3)	0.0162 (3)	0.0138 (3)	0.0013 (3)	0.0044 (2)	0.0012 (3)
O1	0.0119 (8)	0.0220 (10)	0.0201 (10)	0.0049 (9)	0.0064 (7)	0.0009 (9)
O2	0.0242 (10)	0.0133 (9)	0.0209 (11)	0.0000 (8)	0.0102 (9)	0.0042 (8)
O3	0.0376 (12)	0.0285 (12)	0.0288 (13)	−0.0115 (10)	0.0095 (10)	−0.0019 (10)
O4	0.0157 (9)	0.0515 (15)	0.0329 (13)	−0.0051 (10)	0.0109 (9)	0.0064 (12)
O5	0.0194 (10)	0.0153 (9)	0.0158 (10)	0.0043 (8)	0.0067 (8)	0.0053 (8)
O6	0.0099 (8)	0.0269 (11)	0.0190 (10)	0.0008 (9)	0.0061 (7)	0.0016 (9)
O7	0.0378 (13)	0.0292 (13)	0.0329 (13)	−0.0111 (10)	0.0101 (11)	−0.0060 (10)
O8	0.0180 (10)	0.0689 (18)	0.0274 (13)	−0.0077 (11)	0.0114 (10)	0.0055 (12)
N1	0.0135 (11)	0.0249 (12)	0.0184 (12)	0.0064 (10)	0.0067 (9)	0.0022 (10)
N2	0.0116 (10)	0.0147 (11)	0.0196 (12)	0.0000 (9)	0.0078 (9)	−0.0001 (9)
N3	0.0209 (12)	0.0263 (14)	0.0176 (13)	−0.0040 (11)	0.0057 (10)	0.0071 (10)
N4	0.0148 (11)	0.0224 (13)	0.0179 (12)	0.0020 (10)	0.0072 (9)	0.0009 (10)

N5	0.0108 (10)	0.0177 (11)	0.0144 (11)	−0.0028 (9)	0.0046 (9)	−0.0035 (9)
N6	0.0193 (12)	0.0354 (15)	0.0146 (12)	−0.0067 (11)	0.0054 (10)	0.0064 (11)
C1	0.0123 (11)	0.0178 (13)	0.0100 (13)	0.0024 (10)	0.0042 (10)	0.0041 (10)
C2	0.0166 (11)	0.0179 (12)	0.0164 (13)	−0.0044 (12)	0.0062 (10)	0.0015 (12)
C3	0.0177 (13)	0.0173 (14)	0.0217 (15)	0.0033 (11)	0.0062 (11)	−0.0025 (11)
C4	0.0133 (12)	0.0214 (14)	0.0181 (14)	−0.0009 (11)	0.0035 (10)	0.0014 (12)
C5	0.0145 (12)	0.0147 (13)	0.0211 (15)	0.0009 (11)	0.0048 (11)	−0.0006 (11)
C6	0.0151 (12)	0.0134 (13)	0.0166 (13)	0.0032 (12)	0.0059 (10)	0.0000 (12)
C7	0.0206 (13)	0.0143 (13)	0.0224 (15)	−0.0036 (11)	0.0075 (12)	0.0006 (11)
C8	0.0252 (15)	0.0225 (15)	0.0224 (16)	−0.0067 (13)	0.0040 (13)	−0.0035 (12)
C9	0.0255 (14)	0.0278 (16)	0.0184 (15)	0.0041 (13)	0.0038 (12)	−0.0030 (12)
C10	0.0236 (14)	0.0239 (15)	0.0178 (15)	0.0041 (12)	0.0106 (12)	0.0047 (12)
C11	0.0103 (11)	0.0175 (13)	0.0217 (15)	0.0013 (10)	0.0062 (11)	0.0027 (11)
C12	0.0152 (12)	0.0125 (12)	0.0083 (12)	0.0024 (10)	0.0038 (10)	0.0017 (10)
C13	0.0168 (12)	0.0141 (13)	0.0183 (14)	−0.0048 (11)	0.0060 (11)	−0.0026 (11)
C14	0.0225 (13)	0.0147 (12)	0.0186 (13)	−0.0018 (12)	0.0087 (11)	−0.0020 (12)
C15	0.0136 (12)	0.0198 (13)	0.0173 (14)	0.0002 (11)	0.0066 (11)	−0.0031 (11)
C16	0.0093 (11)	0.0150 (12)	0.0173 (14)	−0.0026 (10)	0.0051 (10)	−0.0032 (11)
C17	0.0160 (12)	0.0150 (12)	0.0119 (13)	0.0007 (12)	0.0033 (10)	−0.0004 (11)
C18	0.0193 (13)	0.0163 (14)	0.0198 (15)	−0.0015 (12)	0.0084 (12)	0.0037 (12)
C19	0.0262 (15)	0.0190 (15)	0.0202 (15)	−0.0061 (13)	0.0022 (12)	0.0005 (12)
C20	0.0322 (15)	0.0275 (16)	0.0115 (14)	0.0032 (14)	0.0033 (12)	−0.0006 (13)
C21	0.0193 (13)	0.0221 (15)	0.0205 (15)	0.0031 (12)	0.0110 (12)	0.0049 (12)
C22	0.0118 (11)	0.0181 (14)	0.0172 (14)	0.0001 (11)	0.0045 (11)	0.0019 (11)
O9	0.0157 (9)	0.0210 (10)	0.0194 (11)	0.0003 (9)	0.0072 (8)	−0.0056 (10)
O10	0.0170 (9)	0.0221 (10)	0.0215 (11)	0.0022 (9)	0.0057 (8)	0.0043 (10)

Geometric parameters (Å, º)

S1—O2	1.4464 (19)	C6—C11	1.403 (3)
S1—O1	1.4521 (17)	C7—C8	1.394 (4)
S1—N2	1.581 (2)	C7—H7	0.9300
S1—C6	1.787 (3)	C8—C9	1.383 (4)
S2—O5	1.4416 (19)	C8—H8	0.9300
S2—O6	1.4568 (17)	C9—C10	1.377 (4)
S2—N5	1.578 (2)	C9—H9	0.9300
S2—C17	1.787 (3)	C10—C11	1.380 (4)
O3—N3	1.211 (3)	C10—H10	0.9300
O4—N3	1.237 (3)	C12—C16	1.409 (3)
O7—N6	1.221 (3)	C12—C13	1.421 (3)
O8—N6	1.221 (3)	C13—C14	1.362 (3)
N1—C4	1.336 (4)	C13—H13	0.9300
N1—C3	1.345 (3)	C14—H14	0.9300
N1—H1A	0.918 (10)	C15—C16	1.385 (3)
N2—C1	1.367 (3)	C15—H15	0.9300
N3—C11	1.478 (3)	C16—H16	0.9300
N4—C14	1.342 (3)	C17—C18	1.386 (4)
N4—C15	1.344 (3)	C17—C22	1.404 (3)

N4—H4A	0.913 (10)	C18—C19	1.380 (4)
N5—C12	1.365 (3)	C18—H18	0.9300
N6—C22	1.482 (3)	C19—C20	1.379 (4)
C1—C2	1.405 (4)	C19—H19	0.9300
C1—C5	1.419 (4)	C20—C21	1.380 (4)
C2—C3	1.387 (3)	C20—H20	0.9300
C2—H2	0.9300	C21—C22	1.385 (4)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.376 (3)	O9—H9A	0.864 (10)
C4—H4	0.9300	O9—H9B	0.867 (10)
C5—H5	0.9300	O10—H10A	0.867 (10)
C6—C7	1.389 (4)	O10—H10B	0.870 (10)

O2—S1—O1	116.08 (11)	C9—C8—C7	120.3 (3)
O2—S1—N2	114.62 (10)	C9—C8—H8	119.9
O1—S1—N2	106.27 (11)	C7—C8—H8	119.9
O2—S1—C6	105.68 (13)	C10—C9—C8	119.8 (3)
O1—S1—C6	105.03 (11)	C10—C9—H9	120.1
N2—S1—C6	108.55 (13)	C8—C9—H9	120.1
O5—S2—O6	116.29 (11)	C9—C10—C11	119.8 (3)
O5—S2—N5	114.48 (10)	C9—C10—H10	120.1
O6—S2—N5	106.33 (12)	C11—C10—H10	120.1
O5—S2—C17	105.23 (12)	C10—C11—C6	121.9 (3)
O6—S2—C17	105.61 (11)	C10—C11—N3	117.1 (2)
N5—S2—C17	108.33 (12)	C6—C11—N3	121.0 (2)
C4—N1—C3	121.3 (2)	N5—C12—C16	127.0 (2)
C4—N1—H1A	120 (2)	N5—C12—C13	116.4 (2)
C3—N1—H1A	119 (2)	C16—C12—C13	116.6 (2)
C1—N2—S1	123.21 (19)	C14—C13—C12	120.2 (2)
O3—N3—O4	124.9 (3)	C14—C13—H13	119.9
O3—N3—C11	119.3 (2)	C12—C13—H13	119.9
O4—N3—C11	115.9 (2)	N4—C14—C13	121.6 (3)
C14—N4—C15	120.7 (2)	N4—C14—H14	119.2
C14—N4—H4A	118.3 (19)	C13—C14—H14	119.2
C15—N4—H4A	121.0 (19)	N4—C15—C16	120.9 (2)
C12—N5—S2	123.16 (18)	N4—C15—H15	119.6
O7—N6—O8	125.8 (3)	C16—C15—H15	119.6
O7—N6—C22	118.2 (2)	C15—C16—C12	120.0 (2)
O8—N6—C22	115.9 (2)	C15—C16—H16	120.0
N2—C1—C2	116.3 (2)	C12—C16—H16	120.0
N2—C1—C5	127.2 (2)	C18—C17—C22	116.9 (2)
C2—C1—C5	116.5 (2)	C18—C17—S2	119.0 (2)
C3—C2—C1	120.6 (2)	C22—C17—S2	124.1 (2)
C3—C2—H2	119.7	C19—C18—C17	121.1 (2)
C1—C2—H2	119.7	C19—C18—H18	119.4
N1—C3—C2	120.3 (2)	C17—C18—H18	119.4
N1—C3—H3	119.8	C20—C19—C18	121.0 (3)
C2—C3—H3	119.8	C20—C19—H19	119.5

N1—C4—C5	121.1 (3)	C18—C19—H19	119.5
N1—C4—H4	119.5	C19—C20—C21	119.6 (3)
C5—C4—H4	119.5	C19—C20—H20	120.2
C4—C5—C1	120.2 (2)	C21—C20—H20	120.2
C4—C5—H5	119.9	C20—C21—C22	119.1 (3)
C1—C5—H5	119.9	C20—C21—H21	120.4
C7—C6—C11	117.3 (2)	C22—C21—H21	120.4
C7—C6—S1	119.3 (2)	C21—C22—C17	122.3 (2)
C11—C6—S1	123.3 (2)	C21—C22—N6	115.7 (2)
C6—C7—C8	120.9 (3)	C17—C22—N6	122.0 (2)
C6—C7—H7	119.6	H9A—O9—H9B	111.6 (16)
C8—C7—H7	119.6	H10A—O10—H10B	110.7 (16)

O2—S1—N2—C1	36.7 (2)	O4—N3—C11—C10	62.9 (3)
O1—S1—N2—C1	166.3 (2)	O3—N3—C11—C6	64.4 (4)
C6—S1—N2—C1	−81.2 (2)	O4—N3—C11—C6	−116.0 (3)
O5—S2—N5—C12	−36.0 (2)	S2—N5—C12—C16	−4.2 (4)
O6—S2—N5—C12	−165.8 (2)	S2—N5—C12—C13	175.7 (2)
C17—S2—N5—C12	81.0 (2)	N5—C12—C13—C14	−178.5 (2)
S1—N2—C1—C2	−178.07 (19)	C16—C12—C13—C14	1.4 (4)
S1—N2—C1—C5	1.5 (4)	C15—N4—C14—C13	−0.6 (4)
N2—C1—C2—C3	177.8 (2)	C12—C13—C14—N4	−0.4 (4)
C5—C1—C2—C3	−1.9 (4)	C14—N4—C15—C16	0.6 (4)
C4—N1—C3—C2	−0.8 (4)	N4—C15—C16—C12	0.4 (4)
C1—C2—C3—N1	1.4 (4)	N5—C12—C16—C15	178.5 (2)
C3—N1—C4—C5	0.7 (4)	C13—C12—C16—C15	−1.3 (4)
N1—C4—C5—C1	−1.2 (4)	O5—S2—C17—C18	18.6 (2)
N2—C1—C5—C4	−177.8 (3)	O6—S2—C17—C18	142.2 (2)
C2—C1—C5—C4	1.8 (4)	N5—S2—C17—C18	−104.2 (2)
O2—S1—C6—C7	−14.8 (2)	O5—S2—C17—C22	−159.0 (2)
O1—S1—C6—C7	−138.0 (2)	O6—S2—C17—C22	−35.5 (3)
N2—S1—C6—C7	108.6 (2)	N5—S2—C17—C22	78.1 (2)
O2—S1—C6—C11	161.6 (2)	C22—C17—C18—C19	−1.0 (4)
O1—S1—C6—C11	38.3 (3)	S2—C17—C18—C19	−178.8 (2)
N2—S1—C6—C11	−75.0 (2)	C17—C18—C19—C20	1.1 (4)
C11—C6—C7—C8	0.6 (4)	C18—C19—C20—C21	0.1 (4)
S1—C6—C7—C8	177.2 (2)	C19—C20—C21—C22	−1.2 (4)
C6—C7—C8—C9	−0.1 (4)	C20—C21—C22—C17	1.3 (4)
C7—C8—C9—C10	−1.1 (4)	C20—C21—C22—N6	−179.0 (2)
C8—C9—C10—C11	1.7 (4)	C18—C17—C22—C21	−0.2 (4)
C9—C10—C11—C6	−1.2 (4)	S2—C17—C22—C21	177.5 (2)
C9—C10—C11—N3	180.0 (2)	C18—C17—C22—N6	−179.9 (2)
C7—C6—C11—C10	0.0 (4)	S2—C17—C22—N6	−2.2 (4)
S1—C6—C11—C10	−176.4 (2)	O7—N6—C22—C21	116.6 (3)
C7—C6—C11—N3	178.8 (2)	O8—N6—C22—C21	−62.4 (3)
S1—C6—C11—N3	2.4 (4)	O7—N6—C22—C17	−63.7 (4)
O3—N3—C11—C10	−116.7 (3)	O8—N6—C22—C17	117.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O9	0.91 (1)	1.87 (1)	2.764 (3)	167 (3)
O9—H9*A*···O1	0.86 (1)	2.12 (1)	2.967 (3)	166 (3)
N1—H1*A*···O10^{i}	0.92 (1)	1.84 (1)	2.757 (3)	174 (4)
O9—H9*B*···N5^{ii}	0.87 (1)	2.04 (1)	2.901 (3)	170 (2)
O9—H9*B*···O6^{ii}	0.87 (1)	2.56 (2)	3.125 (3)	123 (2)
O10—H10*A*···O6^{iii}	0.87 (1)	2.05 (1)	2.914 (3)	174 (4)
O10—H10*B*···N2^{iv}	0.87 (1)	2.04 (1)	2.902 (3)	170 (3)

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