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

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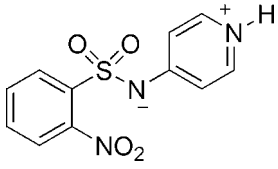
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; R factor = 0.058; wR factor = 0.174; data-to-parameter ratio = 12.5.

The title compound, $C_{11}H_9N_3O_4S$, crystallizes with two molecules in the asymmetric unit; each molecule exists as a zwitterion in the solid state. Intermolecular N—H···N hydrogen bonds link the molecules into chains. Weak C—H···O interactions further stabilize the crystal structure.

Related literature

For zwitterionic forms of *N*-arylbenzenesulfonamides, see: Yu *et al.* (2007); Amendola *et al.*(2005); Lindley *et al.* (1977); Schaumann *et al.* (1975).



Experimental

Crystal data

$C_{11}H_9N_3O_4S$
M_r = 279.27
Triclinic, $P\overline{1}$
a = 7.768 (3) Å
b = 12.570 (5) Å
c = 13.436 (5) Å
α = 75.534 (7)°
β = 85.400 (7)°
γ = 88.741 (6)°
V = 1266.3 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 294 (2) K
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.924, T_{max} = 0.948
6351 measured reflections
4357 independent reflections
2918 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.174
S = 1.02
4357 reflections
349 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O1^{i}	0.95 (4)	2.67 (4)	3.215 (4)	117 (3)
N4—H4A···N2^{i}	0.95 (4)	2.08 (4)	2.969 (4)	155 (3)
N1—H1A···N5^{ii}	0.88 (5)	2.02 (5)	2.898 (4)	172 (4)
C14—H14···O1^{i}	0.93	2.54	3.140 (5)	122
C14—H14···O6^{iii}	0.93	2.58	3.249 (5)	130
C16—H16···O1^{iv}	0.93	2.54	3.265 (5)	135

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2635).

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supporting information

Acta Cryst. (2008). E**64**, o204 [https://doi.org/10.1107/S1600536807064410]

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

Jiang-Sheng Li, Dao-Wu Yang and Wei-Dong Liu

S1. Comment

The title compound crystallizes with two molecules in the asymmetric unit; each molecule displays a zwitterion structure with the pyridine N protonated and the amide N deprotonated (Figs. 1 and 2). The relatively short C1—N2 [1.382 (4) Å] and C12—N5 [1.374 (4) Å] distances indicate that the N2 and N5 lone-pair electrons weakly conjugate with pyridinium rings. The benzene ring forms an angle of 85.1 (2) and 89.3 (2)° with the pyridinium ring in the two molecules of the asymmetric unit. In the addition, the nitro group is inclined to the benzene ring with 73.3 (3)°, and 80.0 (4)°. In the crystal, intermolecular N—H···N and C—H···O hydrogen bonds (Table 1) link the molecules into chains.

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 stirring overnight. The yellow solid obtained was washed with warm water in a yield of 70.3%. Yellow blocks were grown from its formic solution.

S3. Refinement

The N-bound H atoms were located in a difference map and their coordinates were refined with U_{iso}(H) = 1.2 U_{eq}(N). The C-bound H atoms were positioned geometrically (C—H =0.93 Å) and refined as riding with U_{iso}(H) = 1.2 U_{eq}(C).

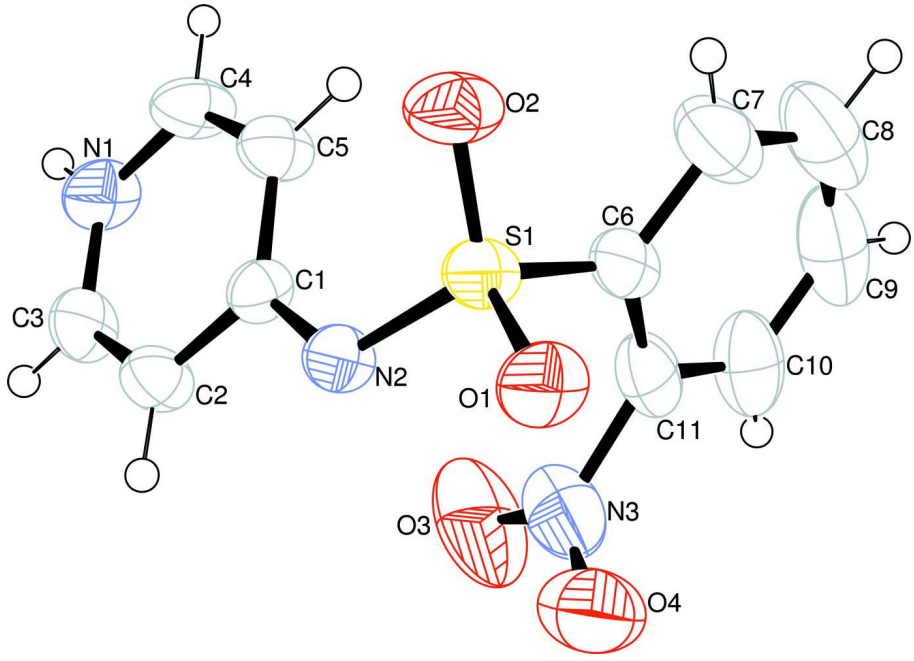

Figure 1

Perspective view of one of the two molecules in the asymmetric unit with the atom-numbering scheme and 50% probability displacement ellipsoids.

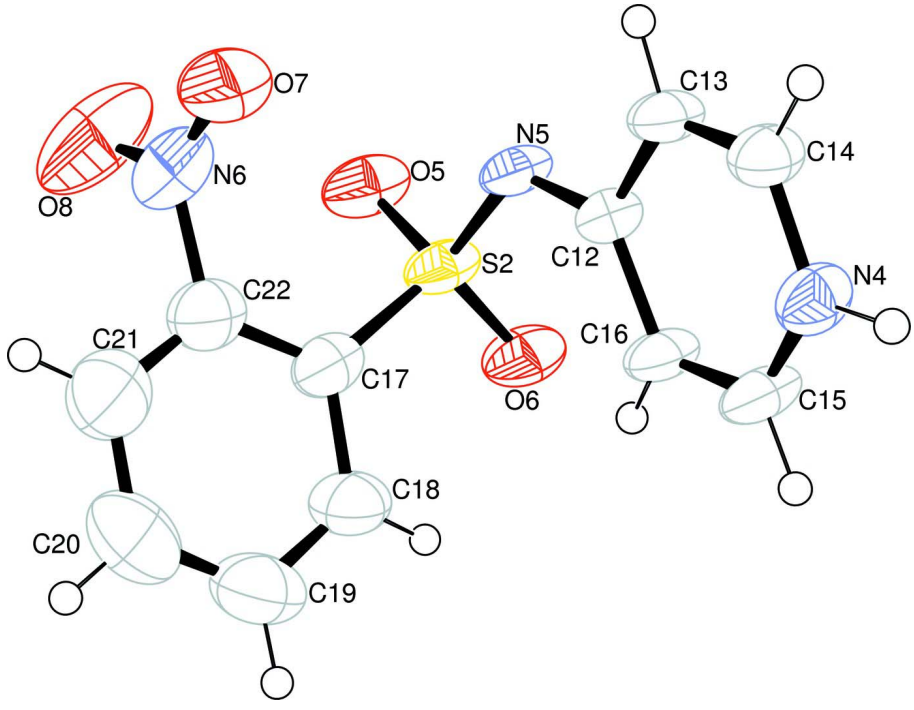

Figure 2

Perspective view of the other molecule in the asymmetric unit with the atom-numbering scheme and 50% probability displacement ellipsoids.

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

Crystal data

$C_{11}H_9N_3O_4S$
$M_r = 279.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.768$ (3) Å
$b = 12.570$ (5) Å
$c = 13.436$ (5) Å
$\alpha = 75.534$ (7)°
$\beta = 85.400$ (7)°
$\gamma = 88.741$ (6)°
$V = 1266.3$ (8) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.465$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2204 reflections
$\theta = 3.0$–$24.8°$
$\mu = 0.27$ mm^{-1}
$T = 294$ K
Block, yellow
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.924$, $T_{max} = 0.948$
6351 measured reflections
4357 independent reflections
2918 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -9 \rightarrow 8$
$k = -14 \rightarrow 11$
$l = -15 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.174$
$S = 1.02$
4357 reflections
349 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2 + 0.7778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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	0.35624 (11)	1.06378 (7)	0.83977 (8)	0.0438 (3)
S2	0.16866 (12)	0.54595 (7)	0.82807 (9)	0.0484 (3)
O1	0.3338 (3)	1.1734 (2)	0.8574 (2)	0.0530 (7)

O2	0.2218 (3)	0.9840 (2)	0.8878 (2)	0.0605 (8)
O3	0.7821 (5)	1.1047 (4)	0.6529 (3)	0.1145 (16)
O4	0.6473 (5)	1.2478 (4)	0.6875 (3)	0.0885 (12)
O5	0.1958 (4)	0.6616 (2)	0.8216 (3)	0.0646 (9)
O6	0.2869 (3)	0.4682 (2)	0.8871 (2)	0.0619 (8)
O7	−0.1188 (6)	0.6900 (4)	0.6559 (3)	0.1066 (15)
O8	0.1034 (8)	0.7942 (3)	0.6026 (4)	0.141 (2)
N1	0.7802 (4)	0.7241 (3)	0.8638 (3)	0.0519 (9)
H1A	0.828 (6)	0.660 (4)	0.864 (3)	0.062*
N2	0.5495 (4)	1.0267 (2)	0.8668 (2)	0.0408 (7)
N3	0.6518 (5)	1.1607 (4)	0.6602 (3)	0.0714 (11)
N4	−0.2797 (4)	0.2206 (3)	0.9043 (3)	0.0471 (8)
H4A	−0.344 (5)	0.154 (3)	0.914 (3)	0.056*
N5	−0.0324 (4)	0.5224 (2)	0.8627 (3)	0.0439 (8)
N6	0.0329 (7)	0.7048 (4)	0.6261 (4)	0.0840 (13)
C1	0.6149 (4)	0.9243 (3)	0.8638 (3)	0.0367 (8)
C2	0.7930 (5)	0.9064 (3)	0.8816 (3)	0.0467 (10)
H2	0.8574	0.9625	0.8941	0.056*
C3	0.8711 (5)	0.8074 (3)	0.8804 (3)	0.0498 (10)
H3	0.9878	0.7978	0.8910	0.060*
C4	0.6109 (5)	0.7371 (3)	0.8454 (3)	0.0529 (11)
H4	0.5509	0.6790	0.8332	0.063*
C5	0.5256 (5)	0.8354 (3)	0.8445 (3)	0.0469 (9)
H5	0.4097	0.8429	0.8311	0.056*
C6	0.3505 (5)	1.0794 (3)	0.7031 (3)	0.0489 (10)
C7	0.2000 (6)	1.0521 (4)	0.6646 (5)	0.0733 (14)
H7	0.1070	1.0224	0.7104	0.088*
C8	0.1865 (8)	1.0684 (5)	0.5589 (6)	0.0930 (19)
H8	0.0834	1.0522	0.5352	0.112*
C9	0.3248 (9)	1.1085 (5)	0.4890 (5)	0.0883 (19)
H9	0.3158	1.1162	0.4190	0.106*
C10	0.4776 (7)	1.1375 (4)	0.5235 (4)	0.0729 (14)
H10	0.5709	1.1654	0.4773	0.088*
C11	0.4862 (5)	1.1233 (3)	0.6295 (3)	0.0535 (11)
C12	−0.1050 (5)	0.4203 (3)	0.8786 (3)	0.0387 (8)
C13	−0.2877 (4)	0.4112 (3)	0.8968 (3)	0.0435 (9)
H13	−0.3524	0.4731	0.9014	0.052*
C14	−0.3706 (5)	0.3136 (3)	0.9076 (3)	0.0445 (9)
H14	−0.4905	0.3107	0.9174	0.053*
C15	−0.1061 (5)	0.2233 (3)	0.8910 (3)	0.0494 (10)
H15	−0.0461	0.1586	0.8906	0.059*
C16	−0.0145 (5)	0.3191 (3)	0.8780 (3)	0.0452 (9)
H16	0.1054	0.3184	0.8689	0.054*
C17	0.1985 (5)	0.5308 (3)	0.6978 (3)	0.0510 (10)
C18	0.2909 (6)	0.4405 (4)	0.6757 (4)	0.0650 (12)
H18	0.3386	0.3891	0.7288	0.078*
C19	0.3118 (7)	0.4269 (5)	0.5753 (4)	0.0785 (15)
H19	0.3684	0.3649	0.5631	0.094*

C20	0.2496 (7)	0.5043 (5)	0.4941 (5)	0.0835 (16)
H20	0.2678	0.4960	0.4272	0.100*
C21	0.1591 (7)	0.5951 (5)	0.5133 (4)	0.0792 (15)
H21	0.1146	0.6473	0.4596	0.095*
C22	0.1365 (6)	0.6065 (4)	0.6129 (4)	0.0609 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0292 (5)	0.0336 (5)	0.0692 (7)	0.0070 (4)	−0.0021 (4)	−0.0151 (4)
S2	0.0308 (5)	0.0362 (5)	0.0800 (8)	0.0050 (4)	−0.0071 (5)	−0.0173 (5)
O1	0.0437 (15)	0.0371 (14)	0.080 (2)	0.0118 (12)	−0.0007 (13)	−0.0210 (13)
O2	0.0355 (15)	0.0474 (16)	0.096 (2)	−0.0039 (12)	0.0047 (14)	−0.0152 (14)
O3	0.042 (2)	0.187 (5)	0.107 (3)	0.030 (3)	−0.0068 (19)	−0.025 (3)
O4	0.094 (3)	0.098 (3)	0.073 (2)	−0.037 (2)	−0.0075 (19)	−0.016 (2)
O5	0.0410 (16)	0.0427 (16)	0.114 (3)	−0.0023 (12)	−0.0067 (16)	−0.0272 (16)
O6	0.0389 (16)	0.0580 (18)	0.091 (2)	0.0156 (13)	−0.0159 (14)	−0.0204 (15)
O7	0.102 (3)	0.114 (3)	0.088 (3)	0.060 (3)	0.004 (2)	−0.005 (2)
O8	0.167 (5)	0.049 (2)	0.198 (5)	0.014 (3)	−0.043 (4)	−0.007 (3)
N1	0.047 (2)	0.0334 (18)	0.076 (3)	0.0107 (15)	−0.0029 (17)	−0.0165 (16)
N2	0.0327 (16)	0.0312 (16)	0.061 (2)	0.0069 (12)	−0.0074 (14)	−0.0149 (14)
N3	0.052 (3)	0.106 (4)	0.051 (2)	−0.006 (2)	−0.0016 (18)	−0.009 (2)
N4	0.0427 (19)	0.0346 (17)	0.064 (2)	−0.0025 (14)	−0.0061 (16)	−0.0116 (15)
N5	0.0337 (17)	0.0295 (16)	0.069 (2)	0.0076 (13)	−0.0044 (14)	−0.0143 (14)
N6	0.090 (4)	0.068 (3)	0.083 (3)	0.025 (3)	−0.012 (3)	0.001 (2)
C1	0.0348 (19)	0.0311 (18)	0.043 (2)	0.0036 (15)	−0.0001 (15)	−0.0084 (15)
C2	0.043 (2)	0.038 (2)	0.064 (3)	0.0032 (17)	−0.0134 (19)	−0.0195 (18)
C3	0.040 (2)	0.044 (2)	0.067 (3)	0.0144 (18)	−0.0130 (19)	−0.0144 (19)
C4	0.042 (2)	0.033 (2)	0.088 (3)	0.0000 (17)	−0.003 (2)	−0.023 (2)
C5	0.033 (2)	0.039 (2)	0.070 (3)	0.0034 (16)	−0.0053 (18)	−0.0173 (18)
C6	0.033 (2)	0.033 (2)	0.084 (3)	0.0124 (16)	−0.016 (2)	−0.0191 (19)
C7	0.050 (3)	0.073 (3)	0.106 (4)	0.008 (2)	−0.025 (3)	−0.033 (3)
C8	0.079 (4)	0.104 (5)	0.116 (5)	0.022 (3)	−0.053 (4)	−0.053 (4)
C9	0.109 (5)	0.093 (4)	0.082 (4)	0.051 (4)	−0.051 (4)	−0.049 (3)
C10	0.075 (3)	0.079 (3)	0.068 (3)	0.034 (3)	−0.019 (3)	−0.024 (3)
C11	0.047 (2)	0.057 (3)	0.061 (3)	0.017 (2)	−0.018 (2)	−0.022 (2)
C12	0.039 (2)	0.0328 (19)	0.046 (2)	0.0066 (15)	−0.0058 (16)	−0.0128 (16)
C13	0.032 (2)	0.037 (2)	0.064 (3)	0.0085 (15)	−0.0013 (17)	−0.0165 (17)
C14	0.034 (2)	0.041 (2)	0.059 (3)	0.0043 (16)	−0.0023 (17)	−0.0135 (18)
C15	0.044 (2)	0.031 (2)	0.075 (3)	0.0121 (17)	−0.0098 (19)	−0.0155 (18)
C16	0.0316 (19)	0.033 (2)	0.071 (3)	0.0094 (15)	−0.0041 (17)	−0.0143 (18)
C17	0.033 (2)	0.036 (2)	0.079 (3)	−0.0037 (16)	0.0024 (19)	−0.0073 (19)
C18	0.051 (3)	0.061 (3)	0.081 (4)	0.011 (2)	0.008 (2)	−0.018 (2)
C19	0.067 (3)	0.079 (4)	0.093 (4)	0.006 (3)	0.016 (3)	−0.034 (3)
C20	0.065 (3)	0.106 (5)	0.080 (4)	−0.015 (3)	0.018 (3)	−0.029 (3)
C21	0.061 (3)	0.077 (4)	0.089 (4)	−0.003 (3)	0.005 (3)	−0.004 (3)
C22	0.053 (3)	0.049 (3)	0.077 (3)	−0.003 (2)	0.004 (2)	−0.014 (2)

Geometric parameters (Å, º)

S1—O2	1.459 (3)	C5—H5	0.9300
S1—O1	1.460 (3)	C6—C7	1.399 (6)
S1—N2	1.605 (3)	C6—C11	1.407 (6)
S1—C6	1.801 (5)	C7—C8	1.395 (8)
S2—O5	1.453 (3)	C7—H7	0.9300
S2—O6	1.455 (3)	C8—C9	1.384 (9)
S2—N5	1.606 (3)	C8—H8	0.9300
S2—C17	1.804 (5)	C9—C10	1.396 (8)
O3—N3	1.232 (5)	C9—H9	0.9300
O4—N3	1.237 (5)	C10—C11	1.397 (6)
O7—N6	1.217 (6)	C10—H10	0.9300
O8—N6	1.219 (6)	C12—C13	1.423 (5)
N1—C3	1.348 (5)	C12—C16	1.441 (5)
N1—C4	1.356 (5)	C13—C14	1.368 (5)
N1—H1A	0.88 (5)	C13—H13	0.9300
N2—C1	1.382 (4)	C14—H14	0.9300
N3—C11	1.501 (6)	C15—C16	1.377 (5)
N4—C15	1.346 (5)	C15—H15	0.9300
N4—C14	1.360 (5)	C16—H16	0.9300
N4—H4A	0.95 (4)	C17—C22	1.402 (6)
N5—C12	1.374 (4)	C17—C18	1.411 (6)
N6—C22	1.499 (6)	C18—C19	1.397 (7)
C1—C5	1.416 (5)	C18—H18	0.9300
C1—C2	1.427 (5)	C19—C20	1.380 (8)
C2—C3	1.376 (5)	C19—H19	0.9300
C2—H2	0.9300	C20—C21	1.396 (7)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.387 (5)	C21—C22	1.378 (7)
C4—H4	0.9300	C21—H21	0.9300
O2—S1—O1	116.20 (17)	C6—C7—H7	119.3
O2—S1—N2	115.50 (16)	C9—C8—C7	120.7 (5)
O1—S1—N2	106.12 (15)	C9—C8—H8	119.6
O2—S1—C6	105.37 (18)	C7—C8—H8	119.6
O1—S1—C6	106.63 (16)	C8—C9—C10	120.1 (5)
N2—S1—C6	106.27 (16)	C8—C9—H9	120.0
O5—S2—O6	116.83 (17)	C10—C9—H9	120.0
O5—S2—N5	106.34 (16)	C9—C10—C11	118.1 (5)
O6—S2—N5	114.96 (17)	C9—C10—H10	121.0
O5—S2—C17	106.20 (18)	C11—C10—H10	121.0
O6—S2—C17	106.00 (18)	C10—C11—C6	123.5 (4)
N5—S2—C17	105.63 (17)	C10—C11—N3	114.9 (4)
C3—N1—C4	120.7 (3)	C6—C11—N3	121.6 (4)
C3—N1—H1A	122 (3)	N5—C12—C13	118.1 (3)
C4—N1—H1A	117 (3)	N5—C12—C16	126.5 (3)
C1—N2—S1	122.7 (2)	C13—C12—C16	115.4 (3)

O3—N3—O4	125.2 (5)	C14—C13—C12	121.7 (3)
O3—N3—C11	117.7 (5)	C14—C13—H13	119.2
O4—N3—C11	117.1 (4)	C12—C13—H13	119.2
C15—N4—C14	120.3 (3)	N4—C14—C13	120.7 (3)
C15—N4—H4A	122 (2)	N4—C14—H14	119.6
C14—N4—H4A	117 (2)	C13—C14—H14	119.6
C12—N5—S2	122.8 (2)	N4—C15—C16	122.0 (3)
O7—N6—O8	124.3 (5)	N4—C15—H15	119.0
O7—N6—C22	117.2 (5)	C16—C15—H15	119.0
O8—N6—C22	118.4 (5)	C15—C16—C12	119.9 (3)
N2—C1—C5	127.5 (3)	C15—C16—H16	120.1
N2—C1—C2	116.3 (3)	C12—C16—H16	120.1
C5—C1—C2	116.3 (3)	C22—C17—C18	115.8 (4)
C3—C2—C1	121.0 (3)	C22—C17—S2	123.5 (3)
C3—C2—H2	119.5	C18—C17—S2	120.7 (3)
C1—C2—H2	119.5	C19—C18—C17	121.1 (4)
N1—C3—C2	120.7 (4)	C19—C18—H18	119.4
N1—C3—H3	119.6	C17—C18—H18	119.4
C2—C3—H3	119.6	C20—C19—C18	120.8 (5)
N1—C4—C5	121.3 (3)	C20—C19—H19	119.6
N1—C4—H4	119.4	C18—C19—H19	119.6
C5—C4—H4	119.4	C19—C20—C21	119.4 (5)
C4—C5—C1	120.0 (3)	C19—C20—H20	120.3
C4—C5—H5	120.0	C21—C20—H20	120.3
C1—C5—H5	120.0	C22—C21—C20	119.2 (5)
C7—C6—C11	116.2 (4)	C22—C21—H21	120.4
C7—C6—S1	119.4 (4)	C20—C21—H21	120.4
C11—C6—S1	124.3 (3)	C21—C22—C17	123.6 (4)
C8—C7—C6	121.4 (5)	C21—C22—N6	115.2 (4)
C8—C7—H7	119.3	C17—C22—N6	121.2 (4)

O2—S1—N2—C1	46.5 (3)	O4—N3—C11—C10	105.2 (5)
O1—S1—N2—C1	176.9 (3)	O3—N3—C11—C6	108.8 (5)
C6—S1—N2—C1	−69.9 (3)	O4—N3—C11—C6	−73.6 (5)
O5—S2—N5—C12	−178.8 (3)	S2—N5—C12—C13	−172.5 (3)
O6—S2—N5—C12	−47.9 (4)	S2—N5—C12—C16	7.1 (5)
C17—S2—N5—C12	68.6 (3)	N5—C12—C13—C14	176.4 (3)
S1—N2—C1—C5	−4.5 (5)	C16—C12—C13—C14	−3.2 (5)
S1—N2—C1—C2	175.0 (3)	C15—N4—C14—C13	0.5 (6)
N2—C1—C2—C3	180.0 (3)	C12—C13—C14—N4	2.0 (6)
C5—C1—C2—C3	−0.5 (6)	C14—N4—C15—C16	−1.5 (6)
C4—N1—C3—C2	1.7 (6)	N4—C15—C16—C12	0.1 (6)
C1—C2—C3—N1	−1.0 (6)	N5—C12—C16—C15	−177.3 (4)
C3—N1—C4—C5	−0.9 (6)	C13—C12—C16—C15	2.2 (5)
N1—C4—C5—C1	−0.6 (6)	O5—S2—C17—C22	−40.9 (4)
N2—C1—C5—C4	−179.3 (4)	O6—S2—C17—C22	−165.8 (3)
C2—C1—C5—C4	1.2 (5)	N5—S2—C17—C22	71.8 (4)
O2—S1—C6—C7	22.1 (4)	O5—S2—C17—C18	137.9 (3)

O1—S1—C6—C7	−101.9 (3)	O6—S2—C17—C18	13.0 (4)
N2—S1—C6—C7	145.2 (3)	N5—S2—C17—C18	−109.4 (3)
O2—S1—C6—C11	−161.2 (3)	C22—C17—C18—C19	−2.3 (6)
O1—S1—C6—C11	74.7 (3)	S2—C17—C18—C19	178.8 (3)
N2—S1—C6—C11	−38.2 (3)	C17—C18—C19—C20	3.1 (7)
C11—C6—C7—C8	−0.4 (6)	C18—C19—C20—C21	−2.4 (8)
S1—C6—C7—C8	176.5 (4)	C19—C20—C21—C22	1.1 (8)
C6—C7—C8—C9	2.5 (8)	C20—C21—C22—C17	−0.6 (7)
C7—C8—C9—C10	−2.7 (8)	C20—C21—C22—N6	−178.2 (5)
C8—C9—C10—C11	0.8 (7)	C18—C17—C22—C21	1.1 (6)
C9—C10—C11—C6	1.3 (6)	S2—C17—C22—C21	−180.0 (4)
C9—C10—C11—N3	−177.5 (4)	C18—C17—C22—N6	178.6 (4)
C7—C6—C11—C10	−1.5 (6)	S2—C17—C22—N6	−2.5 (6)
S1—C6—C11—C10	−178.3 (3)	O7—N6—C22—C21	98.9 (5)
C7—C6—C11—N3	177.2 (4)	O8—N6—C22—C21	−78.3 (6)
S1—C6—C11—N3	0.5 (6)	O7—N6—C22—C17	−78.8 (6)
O3—N3—C11—C10	−72.4 (5)	O8—N6—C22—C17	104.0 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1^{i}	0.95 (4)	2.67 (4)	3.215 (4)	117 (3)
N4—H4*A*···N2^{i}	0.95 (4)	2.08 (4)	2.969 (4)	155 (3)
N1—H1*A*···N5^{ii}	0.88 (5)	2.02 (5)	2.898 (4)	172 (4)
C14—H14···O1^{i}	0.93	2.54	3.140 (5)	122
C14—H14···O6^{iii}	0.93	2.58	3.249 (5)	130
C16—H16···O1^{iv}	0.93	2.54	3.265 (5)	135

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