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Crystal structure of (*E*)-2-(2-{5-[(2-acetoxyethyl)(methyl)amino]thiophen-2-yl}-vinyl)-3-methylbenzothiazolium iodide monohydrate

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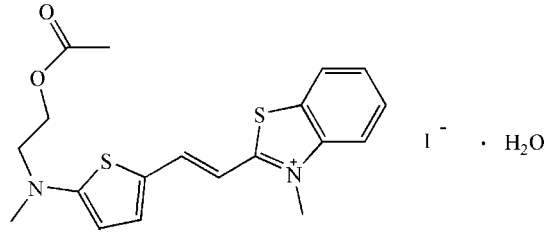
In the cation of the title hydrated salt, $C_{19}H_{21}N_2O_2S_2^+\cdot I^-\cdot H_2O$, the benzothiazolium ring system is approximately planar [maximum deviation = 0.0251 (15) Å], and it makes a small dihedral angle of 1.16 (18)° with the plane of the thiophene ring. In the crystal, the cations, anions and crystalline water molecules are linked by classical O—H···O, O—H···I and weak C—H···O hydrogn bonds, forming a three-dimensional supramolecular network. π–π stacking is observed between parallel thiazole rings of adjacent cations [centroid–centroid distance = 3.5945 (16) Å].

Keywords: crystal structure; benzothiazolium iodide salt; hydrogen bonding.

CCDC reference: 1023218

1. Related literature

Interest in organic compounds with non-linear optical (NLO) properties is driven by the prospective of their applications in optical information technologies. The most common design of molecules with large NLO-activity comprises strong electron donors and acceptors connected by a π-conjugated system, see: Hao *et al.* (2009); Zhou *et al.* (2011). For the crystal structures of related benzothiazolium derivatives, see: Quist *et al.* (2009).



2. Experimental

2.1. Crystal data

$C_{19}H_{21}N_2O_2S_2^+\cdot I^-\cdot H_2O$
M_r = 518.43
Triclinic, $P\overline{1}$
a = 9.6689 (9) Å
b = 11.1237 (11) Å
c = 11.1693 (11) Å
α = 94.420 (1)°
β = 110.067 (1)°
γ = 99.919 (1)°
V = 1099.40 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.67 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.18 mm

2.2. Data collection

Bruker SMART 1000 CCD area-detector diffractometer
8450 measured reflections
4211 independent reflections
3638 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.071
S = 0.97
4211 reflections
247 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···I1^{i}	0.85	2.95	3.647 (3)	140
O2—H2C···O3^{ii}	0.85	2.35	3.056 (5)	140
C7—H7A···O3^{i}	0.96	2.46	3.364 (5)	157
C19—H19A···O2	0.96	2.60	3.554 (6)	173

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5820).

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supporting information

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Crystal structure of (*E*)-2-(2-{5-[(2-acetoxyethyl)(methyl)amino]thiophen-2-yl}vinyl)-3-methylbenzothiazolium iodide monohydrate

Xian-Shun Sun, Ming-Ming Wang and Dan-Dan Li

S1. Comment

Interest in organic compounds with non-linear optical (NLO) properties is driven by the prospective of their applications in optical information technologies. The most common design of molecules with large NLO-active comprises strong electron-donors and acceptors connected by a π-conjugated system (Hao *et al.*, 2009; Zhou *et al.*, 2011). Besides, the introduction about the highpolarizability of sulfur atoms in thiophene rings leads to a stabilization of the conjugated chain and to excellent charge transport properties. In the title compound (I) (Fig. 1), the benzothiazolium-CH═CH-thiophene part of the molecule is nearly coplanar (plane of CH═CH makes angles of 0.663 (8)° and 0.847 (1)° with the planes of the benzothiazolium and the thiophene rings), while in related benzothiazolium derivatives (Quist *et al.* 2009), the corresponding angles are 5.61 (18)° and 1.78 (19)°, respectively.

S2. Experimental

A mixture of 2,3-dimethylbenzothiazolium iodide (1 mmol), 5-[(2-hydroxyethyl)methylamino]thiophene-2-carbaldehyde (1 mmol) and acetic anhydride (20 ml) was refluxed for 20 min, than poured into a warm solution of potassium iodide (4 mmol) in water (20 ml). The precipitated product was filtered, washed with water and recrystallized from a methanol/water solution. ^{1}H NMR: (400 Hz, DMSO-d_6), d(p.p.m.):8.14 (d, 1H), 8.11 (d, 1H), 7.89 (d, 1H), 7.83 (s, 1H), 7.66 (t, 1H), 7.53 (t, 1H), 6.73 (s, 1H), 6.54 (d, 1H), 4.33 (t, 2H), 4.00 (s, 3H), 3.85 (t, 2H), 3.24 (s, 3H), 1.94 (s, 3H).

S3. Refinement

All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with O—H = 0.85, C—H = 0.93–0.97 Å, U_{iso}(H) = 1.5U_{eq}(C,O) for methyl H and water H atoms, and 1.2U_{eq}(C) for the others.

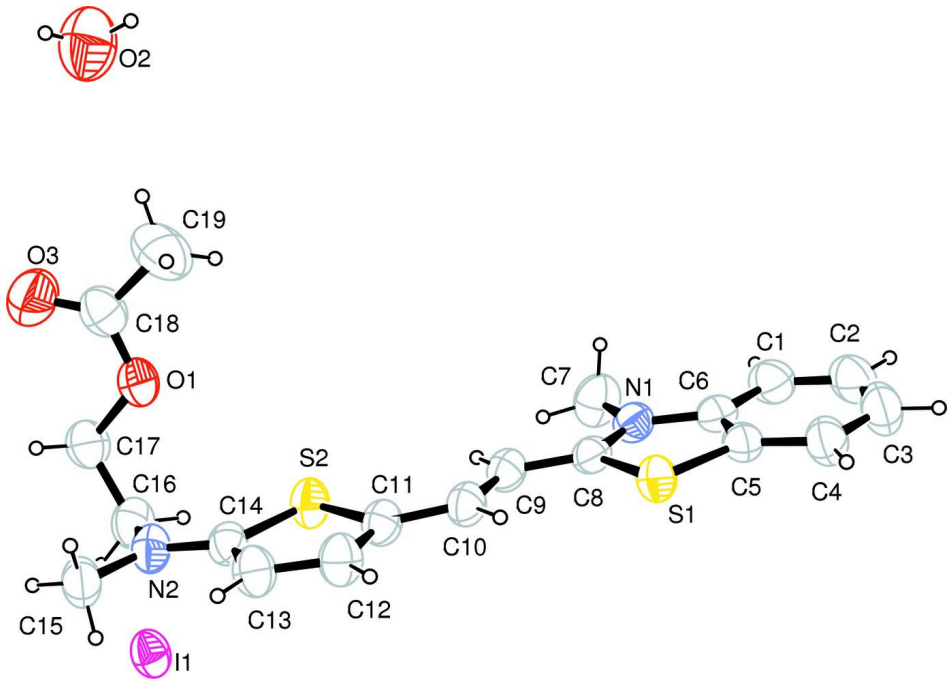

Figure 1

The molecular structure of the title compound (I) showing 30% probability displacement ellipsoids.

(*E*)-2-(2-{5-[(2-Acetoxyethyl)(methyl)amino]thiophen-2-yl}vinyl)-3-methylbenzothiazolium iodide monohydrate

Crystal data

$C_{19}H_{21}N_2O_2S_2^+ \cdot I^- \cdot H_2O$
$M_r = 518.43$
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$\beta = 110.067\ (1)°$
$\gamma = 99.919\ (1)°$
$V = 1099.40\ (18)$ Å^3
$Z = 2$
$F(000) = 520$
$D_x = 1.566$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3223 reflections
$\theta = 2.6–26.8°$
$\mu = 1.67$ mm^{-1}
$T = 293$ K
Block, red
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
8450 measured reflections
4211 independent reflections
3638 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
$h = -11\rightarrow11$
$k = -13\rightarrow13$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.071$
$S = 0.97$
4211 reflections
247 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
$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.5766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8392 (4)	1.1137 (3)	1.1880 (3)	0.0617 (8)
H1	0.9151	1.1225	1.1540	0.074*
C2	0.8380 (4)	1.2036 (3)	1.2804 (4)	0.0735 (10)
H2	0.9138	1.2747	1.3076	0.088*
C3	0.7274 (4)	1.1903 (3)	1.3330 (3)	0.0710 (9)
H3	0.7318	1.2513	1.3968	0.085*
C4	0.6105 (4)	1.0881 (3)	1.2926 (3)	0.0608 (8)
H4	0.5353	1.0797	1.3274	0.073*
C5	0.6088 (3)	0.9985 (2)	1.1986 (3)	0.0476 (6)
C6	0.7227 (3)	1.0101 (3)	1.1481 (3)	0.0483 (6)
C7	0.8124 (4)	0.8983 (3)	0.9953 (3)	0.0698 (9)
H7A	0.7863	0.8181	0.9452	0.105*
H7B	0.9112	0.9100	1.0600	0.105*
H7C	0.8113	0.9604	0.9401	0.105*
C8	0.5782 (3)	0.8216 (2)	1.0354 (2)	0.0432 (6)
C9	0.5304 (3)	0.7106 (3)	0.9491 (3)	0.0481 (6)
H9	0.5890	0.6925	0.9021	0.058*
C10	0.4006 (3)	0.6289 (3)	0.9325 (3)	0.0485 (6)
H10	0.3468	0.6512	0.9824	0.058*
C11	0.3379 (3)	0.5172 (3)	0.8514 (3)	0.0498 (6)
C12	0.2052 (3)	0.4370 (3)	0.8388 (3)	0.0565 (7)
H12	0.1471	0.4533	0.8869	0.068*
C13	0.1650 (3)	0.3322 (3)	0.7507 (3)	0.0553 (7)
H13	0.0780	0.2720	0.7329	0.066*
C14	0.2699 (3)	0.3259 (3)	0.6907 (3)	0.0481 (6)

C15	0.1367 (4)	0.1291 (3)	0.5589 (3)	0.0627 (8)
H15A	0.1256	0.0933	0.6314	0.094*
H15B	0.1532	0.0685	0.5022	0.094*
H15C	0.0469	0.1569	0.5134	0.094*
C16	0.3834 (4)	0.2325 (3)	0.5509 (3)	0.0616 (8)
H16A	0.4097	0.1522	0.5533	0.074*
H16B	0.4725	0.2934	0.6045	0.074*
C17	0.3371 (4)	0.2598 (3)	0.4147 (3)	0.0679 (9)
H17A	0.4175	0.2563	0.3821	0.081*
H17B	0.2482	0.1996	0.3597	0.081*
C18	0.2295 (4)	0.4128 (3)	0.3042 (4)	0.0652 (9)
C19	0.1969 (5)	0.5379 (4)	0.3189 (5)	0.1004 (14)
H19A	0.1788	0.5703	0.2390	0.151*
H19B	0.2815	0.5915	0.3852	0.151*
H19C	0.1093	0.5326	0.3420	0.151*
I1	0.77902 (2)	0.097609 (18)	0.70194 (2)	0.06164 (9)
N1	0.7029 (3)	0.9082 (2)	1.0575 (2)	0.0474 (5)
N2	0.2650 (3)	0.2336 (2)	0.6039 (2)	0.0543 (6)
O1	0.3053 (3)	0.38152 (19)	0.4157 (2)	0.0676 (6)
O2	0.0975 (4)	0.6590 (3)	0.0227 (3)	0.1165 (11)
H2A	0.0901	0.7284	0.0548	0.175*
H2C	0.0115	0.6207	−0.0300	0.175*
O3	0.1931 (4)	0.3467 (3)	0.2039 (3)	0.1068 (10)
S1	0.47604 (8)	0.86129 (6)	1.12820 (7)	0.04896 (17)
S2	0.41617 (9)	0.45592 (7)	0.74660 (7)	0.05390 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0601 (19)	0.0565 (18)	0.0615 (19)	0.0025 (15)	0.0177 (16)	0.0112 (15)
C2	0.076 (2)	0.0509 (19)	0.074 (2)	−0.0031 (17)	0.0110 (19)	0.0046 (16)
C3	0.081 (2)	0.0509 (18)	0.070 (2)	0.0110 (17)	0.0186 (19)	−0.0075 (16)
C4	0.068 (2)	0.0529 (17)	0.0599 (18)	0.0168 (15)	0.0211 (16)	0.0001 (14)
C5	0.0508 (16)	0.0426 (14)	0.0440 (15)	0.0127 (12)	0.0091 (12)	0.0068 (12)
C6	0.0536 (16)	0.0468 (15)	0.0409 (14)	0.0120 (13)	0.0110 (12)	0.0107 (12)
C7	0.066 (2)	0.082 (2)	0.066 (2)	0.0033 (18)	0.0367 (17)	0.0024 (17)
C8	0.0467 (15)	0.0472 (15)	0.0371 (13)	0.0148 (12)	0.0143 (11)	0.0091 (11)
C9	0.0509 (16)	0.0527 (16)	0.0423 (14)	0.0135 (13)	0.0187 (12)	0.0030 (12)
C10	0.0521 (16)	0.0505 (15)	0.0436 (15)	0.0154 (13)	0.0172 (12)	0.0015 (12)
C11	0.0511 (16)	0.0530 (16)	0.0466 (15)	0.0145 (13)	0.0192 (13)	0.0008 (12)
C12	0.0516 (17)	0.0603 (18)	0.0597 (18)	0.0108 (14)	0.0255 (14)	−0.0024 (14)
C13	0.0455 (16)	0.0543 (17)	0.0610 (18)	0.0055 (13)	0.0174 (14)	−0.0010 (14)
C14	0.0468 (15)	0.0492 (15)	0.0424 (14)	0.0137 (13)	0.0080 (12)	0.0025 (12)
C15	0.067 (2)	0.0493 (17)	0.0566 (18)	0.0091 (15)	0.0084 (15)	−0.0061 (14)
C16	0.0627 (19)	0.0632 (19)	0.0597 (18)	0.0244 (16)	0.0203 (15)	−0.0024 (15)
C17	0.097 (3)	0.0546 (18)	0.063 (2)	0.0304 (18)	0.0367 (19)	0.0014 (15)
C18	0.067 (2)	0.0576 (19)	0.076 (2)	0.0120 (16)	0.0336 (19)	0.0065 (18)
C19	0.114 (4)	0.069 (2)	0.126 (4)	0.039 (2)	0.042 (3)	0.019 (2)

I1	0.06545 (15)	0.05325 (13)	0.06963 (15)	0.00855 (9)	0.03333 (11)	−0.00352 (9)
N1	0.0494 (13)	0.0504 (13)	0.0425 (12)	0.0090 (11)	0.0174 (10)	0.0077 (10)
N2	0.0555 (14)	0.0523 (14)	0.0496 (13)	0.0115 (11)	0.0149 (11)	−0.0053 (11)
O1	0.0943 (17)	0.0500 (12)	0.0587 (13)	0.0227 (12)	0.0266 (12)	−0.0024 (10)
O2	0.121 (3)	0.121 (3)	0.106 (2)	0.028 (2)	0.044 (2)	−0.013 (2)
O3	0.150 (3)	0.093 (2)	0.0662 (17)	0.045 (2)	0.0181 (18)	−0.0002 (15)
S1	0.0494 (4)	0.0476 (4)	0.0501 (4)	0.0109 (3)	0.0197 (3)	−0.0004 (3)
S2	0.0526 (4)	0.0543 (4)	0.0534 (4)	0.0047 (3)	0.0237 (3)	−0.0065 (3)

Geometric parameters (Å, º)

C1—C2	1.384 (5)	C12—C13	1.372 (4)
C1—C6	1.387 (4)	C12—H12	0.9300
C1—H1	0.9300	C13—C14	1.403 (4)
C2—C3	1.379 (5)	C13—H13	0.9300
C2—H2	0.9300	C14—N2	1.340 (3)
C3—C4	1.379 (5)	C14—S2	1.741 (3)
C3—H3	0.9300	C15—N2	1.459 (4)
C4—C5	1.385 (4)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.391 (4)	C15—H15C	0.9600
C5—S1	1.745 (3)	C16—N2	1.459 (4)
C6—N1	1.401 (3)	C16—C17	1.503 (5)
C7—N1	1.465 (4)	C16—H16A	0.9700
C7—H7A	0.9600	C16—H16B	0.9700
C7—H7B	0.9600	C17—O1	1.439 (4)
C7—H7C	0.9600	C17—H17A	0.9700
C8—N1	1.343 (3)	C17—H17B	0.9700
C8—C9	1.408 (4)	C18—O3	1.196 (4)
C8—S1	1.740 (3)	C18—O1	1.318 (4)
C9—C10	1.362 (4)	C18—C19	1.489 (5)
C9—H9	0.9300	C19—H19A	0.9600
C10—C11	1.387 (4)	C19—H19B	0.9600
C10—H10	0.9300	C19—H19C	0.9600
C11—C12	1.387 (4)	O2—H2A	0.8500
C11—S2	1.752 (3)	O2—H2C	0.8500
C2—C1—C6	117.4 (3)	C14—C13—H13	123.8
C2—C1—H1	121.3	N2—C14—C13	126.6 (3)
C6—C1—H1	121.3	N2—C14—S2	122.6 (2)
C3—C2—C1	121.7 (3)	C13—C14—S2	110.8 (2)
C3—C2—H2	119.2	N2—C15—H15A	109.5
C1—C2—H2	119.2	N2—C15—H15B	109.5
C2—C3—C4	121.1 (3)	H15A—C15—H15B	109.5
C2—C3—H3	119.4	N2—C15—H15C	109.5
C4—C3—H3	119.4	H15A—C15—H15C	109.5
C3—C4—C5	117.8 (3)	H15B—C15—H15C	109.5
C3—C4—H4	121.1	N2—C16—C17	112.6 (3)

C5—C4—H4	121.1	N2—C16—H16A	109.1
C4—C5—C6	121.1 (3)	C17—C16—H16A	109.1
C4—C5—S1	128.1 (3)	N2—C16—H16B	109.1
C6—C5—S1	110.7 (2)	C17—C16—H16B	109.1
C1—C6—C5	120.8 (3)	H16A—C16—H16B	107.8
C1—C6—N1	126.9 (3)	O1—C17—C16	107.5 (2)
C5—C6—N1	112.3 (2)	O1—C17—H17A	110.2
N1—C7—H7A	109.5	C16—C17—H17A	110.2
N1—C7—H7B	109.5	O1—C17—H17B	110.2
H7A—C7—H7B	109.5	C16—C17—H17B	110.2
N1—C7—H7C	109.5	H17A—C17—H17B	108.5
H7A—C7—H7C	109.5	O3—C18—O1	122.8 (3)
H7B—C7—H7C	109.5	O3—C18—C19	125.1 (4)
N1—C8—C9	126.3 (2)	O1—C18—C19	112.2 (3)
N1—C8—S1	111.84 (19)	C18—C19—H19A	109.5
C9—C8—S1	121.9 (2)	C18—C19—H19B	109.5
C10—C9—C8	121.8 (2)	H19A—C19—H19B	109.5
C10—C9—H9	119.1	C18—C19—H19C	109.5
C8—C9—H9	119.1	H19A—C19—H19C	109.5
C9—C10—C11	128.8 (3)	H19B—C19—H19C	109.5
C9—C10—H10	115.6	C8—N1—C6	114.3 (2)
C11—C10—H10	115.6	C8—N1—C7	123.9 (2)
C10—C11—C12	126.4 (3)	C6—N1—C7	121.8 (2)
C10—C11—S2	124.4 (2)	C14—N2—C15	119.5 (3)
C12—C11—S2	109.2 (2)	C14—N2—C16	122.8 (3)
C13—C12—C11	115.8 (3)	C15—N2—C16	117.7 (2)
C13—C12—H12	122.1	C18—O1—C17	117.4 (2)
C11—C12—H12	122.1	H2A—O2—H2C	109.5
C12—C13—C14	112.4 (3)	C8—S1—C5	90.83 (14)
C12—C13—H13	123.8	C14—S2—C11	91.88 (14)

C6—C1—C2—C3	1.2 (5)	C9—C8—N1—C7	−1.4 (4)
C1—C2—C3—C4	−2.0 (6)	S1—C8—N1—C7	178.5 (2)
C2—C3—C4—C5	0.8 (5)	C1—C6—N1—C8	−178.9 (3)
C3—C4—C5—C6	1.1 (4)	C5—C6—N1—C8	1.3 (3)
C3—C4—C5—S1	−179.4 (3)	C1—C6—N1—C7	2.1 (4)
C2—C1—C6—C5	0.6 (4)	C5—C6—N1—C7	−177.7 (3)
C2—C1—C6—N1	−179.2 (3)	C13—C14—N2—C15	3.2 (4)
C4—C5—C6—C1	−1.8 (4)	S2—C14—N2—C15	−178.3 (2)
S1—C5—C6—C1	178.6 (2)	C13—C14—N2—C16	−177.0 (3)
C4—C5—C6—N1	178.0 (3)	S2—C14—N2—C16	1.5 (4)
S1—C5—C6—N1	−1.6 (3)	C17—C16—N2—C14	−105.5 (3)
N1—C8—C9—C10	−179.3 (3)	C17—C16—N2—C15	74.3 (4)
S1—C8—C9—C10	0.7 (4)	O3—C18—O1—C17	−3.4 (5)
C8—C9—C10—C11	179.5 (3)	C19—C18—O1—C17	177.0 (3)
C9—C10—C11—C12	179.7 (3)	C16—C17—O1—C18	−164.4 (3)
C9—C10—C11—S2	−0.9 (5)	N1—C8—S1—C5	−0.4 (2)
C10—C11—C12—C13	179.2 (3)	C9—C8—S1—C5	179.6 (2)

S2—C11—C12—C13	−0.3 (4)	C4—C5—S1—C8	−178.4 (3)
C11—C12—C13—C14	0.8 (4)	C6—C5—S1—C8	1.1 (2)
C12—C13—C14—N2	177.7 (3)	N2—C14—S2—C11	−178.0 (2)
C12—C13—C14—S2	−1.0 (3)	C13—C14—S2—C11	0.7 (2)
N2—C16—C17—O1	61.2 (4)	C10—C11—S2—C14	−179.8 (3)
C9—C8—N1—C6	179.6 (3)	C12—C11—S2—C14	−0.3 (2)
S1—C8—N1—C6	−0.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···I1^{i}	0.85	2.95	3.647 (3)	140
O2—H2*C*···O3^{ii}	0.85	2.35	3.056 (5)	140
C7—H7*A*···O3^{i}	0.96	2.46	3.364 (5)	157
C19—H19*A*···O2	0.96	2.60	3.554 (6)	173

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